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LOWER BOUNDS FOR THE RANDIĆ INDEX R_{-1} OF TREES

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Abstract

The Randić index $R_{-1} = R_{-1}(G)$ of a graph G is defined as the sum of the weights $(d_G(u)d_G(v))^{-1}$ of all edges uv of G, where $d_G(u)$ denotes the degree of vertex u. In this paper we give a sharp lower bound for the Randić index R_{-1} of trees with given order and the number of pending vertices, and determine the trees of order $n \geq 6$ with second-minimal, third-minimal and fourth-minimal Randić indices R_{-1}.

INTRODUCTION

Let G be a simple graph. The general Randić index (or connectivity index) of G is defined as

$$R_\alpha = R_\alpha(G) = \sum_{uv} (d_G(u)d_G(v))^\alpha$$

where $d_G(u)$, or simply $d(u)$, denotes the degree of vertex u, α is an arbitrary real number, and the summation goes over all edges of G. Two special cases $\alpha = -1, -1/2$ were introduced by Randić [1] in 1975 in his reasearch on molecular structures. Results on $R_{-1/2}$ can be found in [2–7]. Clark and Moon [8] proved that for a tree T

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with $n \geq 2$ vertices, $1 \leq R_{-1}(T) \leq (5n+8)/18$ with the former equality if and only if T the star S_n, where S_n is the n-vertex tree with maximum degree $n-1$. Hence the tree with minimal Randić index R_{-1} is S_n. Rautenbach [9] gave an upper bound for R_{-1} of trees with maximum degree 3. Recently, Li and Yang [10] obtained a lower bound for R_{-1} of chemical trees.

In this paper we give a lower bound for R_{-1} of trees with given order and the number of pending vertices, and determine the extremal graph. The trees of order $n \geq 6$ with second-minimal, third-minimal and fourth-minimal Randić indices R_{-1} are determined.

MAIN RESULTS

A comet is a tree composed of a star and an appended path. For any positive integer n and n_1 with $2 \leq n_1 \leq n-1$, we denote by $T(n, n_1)$ the comet of order n with n_1 pending vertices, i.e., a tree formed by a path P_{n-n_1} of which one end vertex coincides with a pending vertex of a star of order n_1+1 (see Figure 1).

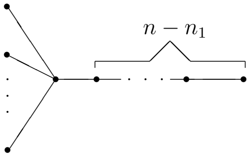

Figure 1. $T(n, n_1)$

We use the techniques in [2]. First we give the following lemma.

Lemma 1. *Let $e = v_1v_2$ be an edge of a tree T of order n with $n_1 \leq n-2$ pending vertices. If $d(v_1) = 1$ and $d(v_2) \geq 2$, then*

$$R_{-1}(T) - R_{-1}(T - v_1) \geq \frac{1}{2n_1(n_1-1)} \tag{1}$$

with equality if and only if T is a comet and v_2 has maximum degree.

Proof. Denote by E_2 the sum of the weights of the edges, other than e, incident with v_2 in T. So by the definition of R_{-1},

$$R_{-1}(T) - R_{-1}(T - v_1) = \frac{1}{d(v_2)} - \frac{E_2}{d(v_2)-1}\,. \tag{2}$$

Since $n_1 \leq n-2$, T is not a star. So at least one vertex adjacent to v_2 has a degree no less than 2. Thus

$$E_2 \leq \frac{1}{2d(v_2)} + (d(v_2)-2)\frac{1}{d(v_2)} = 1 - \frac{3}{2d(v_2)} \tag{3}$$

with equality if and only if all the vertices adjacent to v_2 are pending vertices except one, say v_3, with $d(v_3) = 2$.

By (2), (3) and the fact $d(v_2) \le n_1$, we have

$$\begin{aligned} R_{-1}(T) - R_{-1}(T - v_1) &\ge \frac{1}{d(v_2)} - \frac{1}{d(v_2) - 1}\frac{2d(v_2) - 3}{2d(v_2)} \\ &= \frac{1}{2d(v_2)(d(v_2) - 1)} \ge \frac{1}{2n_1(n_1 - 1)} . \end{aligned}$$

This proves (1). From the above argument, the equality in (1) holds if and only if all the vertices adjacent to v_2 are pending vertices except v_3 with $d(v_3) = 2$ and $d(v_2) = n_1$, i.e., T is a comet and v_2 has maximum degree n_1. □

We now give a lower bound for R_{-1} of trees with given order and the number of pending vertices. The n-vertex path P_n is a tree with maximum degree 2.

Theorem 2. *Let T be a tree of order $n > 3$, with n_1 pending vertices. If $n_1 \le n - 2$, then*

$$R_{-1}(T) \ge 1 - \frac{1}{2n_1} + \frac{n - n_1}{4} \tag{4}$$

with equality if and only if T is the comet $T(n, n_1)$.

Proof. If T is the comet $T(n, n_1)$, it is easy to see that $R_{-1}(T)$ is equal to the right-hand side of (4).

We apply induction on n. Since $n_1 \le n-2$, T is not the star S_n. It can be readily checked that (4) holds when $n = 4, 5$, since these trees are P_4, P_5 and $T(5, 3)$, which are all comets. So we assume that $n \ge 6$ and that the result holds for all smaller values of n.

Let v_1v_2 be a pending edge of T (with $d(v_1) = 1$). There are two cases by discussing the degree of v_2.

Case 1: $d(v_2) = 2$. We denote $v_3 (\ne v_1)$ the other vertex adjacent to v_2 . Since $n \ge 6$, we have $d(v_3) \ge 2$, and then

$$R_{-1}(T) - R_{-1}(T - v_1) = \frac{1}{2} - \frac{1}{2d(v_3)} \ge \frac{1}{4} \tag{5}$$

with equality if and only if $d(v_3) = 2$. As $d(v_2) = 2$, the tree $T - v_1$ has n_1 pending vertices and $n - 1$ vertices. In the case of $n_1 = n - 2$, the tree $T - v_1$ is a star, so T is a comet and we can stop the induction here. If $n_1 \le (n - 1) - 2$, by the induction hypothesis,

$$R_{-1}(T - v_1) \ge 1 - \frac{1}{2n_1} + \frac{n - 1 - n_1}{4} \tag{6}$$

with equality if and only if $T - v_1$ is the comet $T(n-1, n_1)$. So by (5) and (6)

$$R_{-1}(T) \geq 1 - \frac{1}{2n_1} + \frac{n-n_1}{4}$$

with equality if and only if $T - v_1$ is the comet $T(n-1, n_1)$ and $d(v_3) = 2$, i.e., T is the comet $T(n, n_1)$.

Case 2: $d(v_2) \geq 3$. The tree $T - v_1$ has $n_1 - 1$ pending vertices and $n - 1$ vertices. Then, by the induction hypothesis,

$$R_{-1}(T - v_1) \geq 1 - \frac{1}{2(n_1-1)} + \frac{n-n_1}{4} \tag{7}$$

with equality if and only if $T - v_1$ is the comet $T(n-1, n_1 - 1)$. By Lemma 1, we have

$$R_{-1}(T) - R_{-1}(T - v_1) \geq \frac{1}{2n_1(n_1-1)} \tag{8}$$

with equality if and only if T is a comet. Thus, by (7) and (8)

$$R_{-1}(T) \geq 1 - \frac{1}{2n_1} + \frac{n-n_1}{4}$$

with equality if and only if T is the comet $T(n, n_1)$. □

Note that the function

$$f(x) = 1 - \frac{1}{2x} + \frac{n-x}{4}$$

is decreasing for $x \geq 2$. Let T be a tree of order $n > 3$, with n_1 pending vertices. When T is not a star, then $n_1 \leq n - 2$ and by Theorem 2, $R_{-1}(T) \geq f(n-2)$ with equality if and only if T is the comet $T(n, n-2)$. This proves the following.

Corollary 3. *Let T be a tree of order $n \geq 4$. If T is not the star S_n, then*

$$R_{-1}(T) \geq \frac{3}{2} - \frac{1}{2(n-2)}$$

with equality if and only if T is the comet $T(n, n-2)$.

Corollary 4. *Let T be a tree of order n with $n \geq 6$. Suppose that T is neither the star S_n nor the comet $T(n, n-2)$. Then*

$$R_{-1}(T) \geq 1 + \frac{2(n-4)}{3(n-3)}$$

with equality if and only if T is $S_{n,n-4}$ (see Figure 2).

Proof. There are two cases.

Case 1: $n_1 \leq n-3$. By the argument previous to Corollary 3, we have

$$R_{-1}(T) \geq f(n-3) = \frac{7}{4} - \frac{1}{2(n-3)}$$

with equality if and only if T is the comet $T(n, n-3)$.
Case 2: $n_1 = n-2$. Then T is of the form $S_{n,a}$ with $(n-2)/2 \leq a \leq n-4$ (see Figure 2). Obviously, $S_{n,n-3}$ is $T(n, n-2)$.

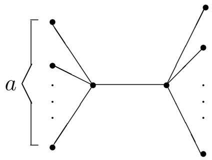

Figure 2. $S_{n,a}$

It is easy to see that

$$R_{-1}(S_{n,a}) = 1 + \frac{a(n-a-2)}{a(n-a-2)+n-1}$$

is decreasing with a when $a \geq (n-2)/2$, and hence

$$R_{-1}(S_{n,n-4}) < R_{-1}(S_{n,n-5}) < \cdots < R_{-1}(S_{n,\lceil (n-2)/2 \rceil}) \ (n \geq 8)\,.$$

It can be readily checked that

$$R_{-1}(S_{n,n-4}) = 1 + \frac{2(n-4)}{3(n-3)} < R_{-1}(T(n, n-3))\,.$$

Then by combining Case 1 and 2, the result follows. □

Note that $R_{-1}(S_{n,n-5}) < R_{-1}(T(n, n-3))$ if $n \geq 8$. From above argument, we also have the following.

Corollary 5. *Let T be a tree of order n with $n \geq 6$. Suppose that T is not the star S_n, the comet $T(n, n-2)$, or $S_{n,n-4}$. Then*

$$R_{-1}(T) \geq 1 + \frac{3(n-5)}{4(n-4)}$$

with equality if and only if T is $S_{n,n-5}$ when $n \geq 8$, and

$$R_{-1}(T) \geq \frac{7}{4} - \frac{1}{2(n-3)}$$

with equality if and only if T is the comet $T(n, n-3)$ when $n = 6, 7$.

By Corollaries 3, 4 and 5, the trees of order $n \geq 6$ with minimal, second-minimal and third-minimal Randić indices R_{-1} are S_n, $T(n, n-2)$ and $S_{n,n-4}$, respectively, and the trees with minimal-fourth Randić indices R_{-1} are $S_{n,n-5}$ for $n \geq 8$ and $T(n, n-3)$ for $n = 6, 7$.

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References

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

[2] P. Hansen, H. Mélot, Variable neighborhood search for extremal graphs, 6. Analyzing bounds for the connectivity index, *J. Chem. Inf. Comput. Sci.* **43** (2003) 1–14.

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

[4] G. Caporossi, I. Gutman, P. Hansen, Variable neighborhood search for extremal graphs IV: Chemical trees with extremal connectivity index, *Comput. Chem.* **23** (1999) 469–477.

[5] I. Gutman, O. Miljković, G. Caporossi, P. Hansen, Alkanes with small and large Randić connectivity indices, *Chem. Phys. Lett.* **306** (1999) 366–372.

[6] O. Araujo, J. A. de la Peña, Some bounds for the connectivity index of a chemical graph, *J. Chem. Inf. Comput. Sci.* **38** (1998) 827–831.

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

[8] L. H. Clark, J. W. Moon, On the general Randić index for certain families of trees, *Ars Combin.* **54** (2000) 223–235.

[9] D. Rautenbach, A note on trees of maximum weight and restricted degrees, *Discrete Math.* **271** (2003) 335–342.

[10] X. Li, Y. Yang, Best lower and upper bounds for the Randić index R_{-1} of chemical trees, *MATCH Commun. Math. Comput. Chem.* **52** (2004) 147–156.