MATCH
Communications in Mathematical
and in Computer Chemistry

no. 52, September 2004
MATCDY (52) 119-128 (2004)

ISSN 0340 - 6253

Trees with minimum general Randić index *

Yumei Hu, Xueliang Li, Yuán Yuan
Center for Combinatorics and LPMC
Nankai University, Tianjin 300071, P.R. China
Email: ym.hu@eyou.com; lxl@nankai.edu.cn; yy.yuan@eyou.com

(Received December 15, 2003)

Abstract

The general Randić index of a (molecular) graph G is defined as the sum of $(d(u)d(v))^\alpha$ over all edges uv of G, where $d(u)$ denotes the degree of a vertex u in G and α is an arbitrary real number. In this paper we show that among trees with n vertices, the path P_n for $\alpha > 0$ and the star S_n for $\alpha < 0$, respectively, has the minimum general Randić index.

Keywords: tree; path; star; general Randić index; minimum

1 Introduction

For a (molecular) graph $G = (V, E)$, the *general Randić index* $R_\alpha(G)$ of G is defined as the sum of $(d_G(u)d_G(v))^\alpha$ over all edges uv of G, where $d_G(u)$ denotes the degree of

*Supported by National Science Foundation of China.

$u \in V$ and α is a real number, i.e.,

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

It is known that the index $R_{-\frac{1}{2}}$ was introduced by Randić [8] in 1975 as one of the many graph-theoretical parameters derived from the graph underlying some molecule. Later, Bollobás and Erdös [1] generalized this index by replacing $-\frac{1}{2}$ by any real number α, which was called the general Randić index. Recently, R_α received considerable attention in the literature, see [2, 4, 5, 6, 10].

Yu [10] gave a sharp upper bound of $R_{-\frac{1}{2}}$ for trees of order n, i.e., $R_{-\frac{1}{2}}(T) \leq \frac{1}{2}(n+2\sqrt{2}-3)$. Bollobás and Erdös [1] gave a sharp upper bound of R_α with $\alpha \in (0,1]$, for graphs of size m, and a sharp lower bound for R_α with $\alpha \in [-1,0)$, also for graphs of size m. Clark and Moon [5] gave several extremal and probabilistic results of R_α for certain families of trees. Li and Yang [7] studied the general Randić index for general graphs, and they obtained lower and upper bounds for the general Randić index among graphs with n vertices, and the corresponding extremal graphs.

Since trees are important molecular structures in chemistry, in the following we only deal with trees, ie., connected graphs without cycles. We give the trees which have the minimum general Randić index, as well as the corresponding values of the index. A clear picture is given depending on the real number α in different intervals.

The set of vertices (edges) of a simple graph G is denoted by $V(G)(E(G))$. The order of G is defined by $|V(G)|$ and the size of G is defined by $|E(G)|$. The *degree* $d(u)$ of a vertex u is the number of vertices adjacent to u in G. A vertex of degree one in a tree is called a *leaf* of that tree. The vertices adjacent to vertex u are called the *neighbors* of u, and the neighborhood of u is denoted by $N(u)$. The *path* of order n is denoted by P_n, and the *star* of order n is denoted by S_n. For $uv \in E(G)$, $w(uv) = (d(u)d(v))^\alpha$ is called the *weight* of uv. Undefined notations and terminology can be found in [3].

For $\alpha = 0$, the general Randić index of any graph G is exactly equal to the size of G, namely $R_0(G) = |E(G)|$. So, for any tree T of order n, we have $R_0(T) = n - 1$.

Therefore, in the following we always assume $\alpha \neq 0$. We distinguish α in two intervals.

2 The case for $\alpha > 0$

Since there are two different non-isomorphic trees with 4 vertices, it is easy to calculate that for μ is proximately equal to 3.0816, if $\alpha > \mu$, S_4 has the minimum value, otherwise P_4 has the minimum value. We assume $n \geq 5$ in the following.

Theorem 2.1 *Among trees with n ($n \geq 5$) vertices, the path P_n has the minimum general Randić index for $\alpha > 0$.*

Proof. Suppose that T is a tree, but not a path, which has the minimum value of the general Randić index for $\alpha > 0$. We will derive contradictions. Suppose that $P = v_1v_2 \ldots v_{k-1}v_k$ is a longest path of T. Then $d(v_1) = d(v_k) = 1$. Considering the degrees of v_2 and v_{k-1}, we distinguish the following two cases.

Case 1. $d(v_2) > 2$ or $d(v_{k-1}) > 2$.

Without loss of generality, we assume that $d(v_{k-1}) = d > 2$. Since P is a longest path of T, all the vertices adjacent to v_{k-1}, other than v_{k-2}, must be leaves. Let $u_1, u_2, \cdots, u_{d-2}$ be the neighbors of v_{k-1}, other than v_{k-2} and v_k. By deleting the edges $v_{k-1}u_1, v_{k-1}u_2, \cdots, v_{k-1}u_{d-2}$ and adding the edges $v_ku_1, v_ku_2, \cdots, v_ku_{d-2}$, we get a new tree T', as shown in Figure 2.1.

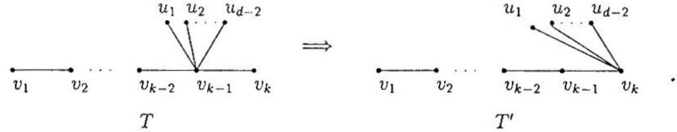

Figure 2.1

If $d(v_{k-2}) = 1$, T is a star S_n. For $n \geq 5$, we have

$$\begin{aligned} R_\alpha(S_n) - R_\alpha(P_n) &= (n-1)^{\alpha+1} - 2^{\alpha+1} - (n-3)4^\alpha \\ &= (n-3)((n-1)^\alpha - 4^\alpha) + 2((n-1)^\alpha - 2^\alpha) > 0. \end{aligned}$$

Now we can assume that $d(v_{k-2}) \geq 2$. So we have

$$\begin{aligned} & R_\alpha(T) - R_\alpha(T') \\ = \ & d(v_{k-2})^\alpha(d^\alpha - 2^\alpha) + d^\alpha - 2^\alpha(d-1)^\alpha + (d-2)d^\alpha - (d-2)(d-1)^\alpha \\ \geq \ & 2^\alpha(d^\alpha - 2^\alpha) + (d-1)d^\alpha - 2^\alpha(d-1)^\alpha - (d-2)(d-1)^\alpha \\ > \ & 2^\alpha(d^\alpha - 2^\alpha) + (d-1)d^\alpha - 2^\alpha(d-1)^\alpha - (d-2)d^\alpha \\ = \ & 2^\alpha(d^\alpha - (d-1)^\alpha) + d^\alpha - 4^\alpha. \end{aligned}$$

Hence, if $d \geq 4$, we have $R_\alpha(T) - R_\alpha(T') > 0$; otherwise, $d = 3$ and then

$$\begin{aligned} R_\alpha(T) - R_\alpha(T') &> 2^\alpha(3^\alpha - 2^\alpha) + 3^\alpha - 4^\alpha \\ &= 6^\alpha + 3^\alpha - 2 \cdot 4^\alpha \\ &\geq 2\sqrt{18^\alpha} - 2\sqrt{16^\alpha} > 0. \end{aligned}$$

Case 2. $d(v_2) = d(v_{k-1}) = 2$.

Since the tree T is not a path, there exists a vertex v_i such that $d(v_i) = d \geq 3$ for some $i = 3, 4, \cdots, k-2$. Let $u_1, u_2, \cdots, u_{d-2}$ be the neighbors of v_i, other than v_{i-1} and v_{i+1}. By deleting edges $u_1v_i, u_2v_i, \cdots, u_{d-2}v_i$ and adding edges $u_1v_k, u_2v_k, \cdots, u_{d-2}v_k$, we get a new tree T' as shown in Figure 2.2.

Denote by S_{v_i} the sum of the weights of the edges adjacent to v_i, other than $v_{i-1}v_i$ and v_iv_{i+1}. Then we have

$$w(v_{i-1}v_i) + w(v_iv_{i+1}) \geq 2 \cdot 2^\alpha d^\alpha \quad and \quad S_{v_i} \geq (d-2)d^\alpha.$$

So,

$$\begin{aligned} & R_\alpha(T) - R_\alpha(T') \\ = \ & (w(v_{i-1}v_i) + w(v_iv_{i+1}))(1 - \frac{2^\alpha}{d^\alpha}) + 2^\alpha(1 - (d-1)^\alpha) + S_{v_i}(1 - (\frac{d-1}{d})^\alpha) \\ \geq \ & 2^{\alpha+1}(d^\alpha - 2^\alpha) + 2^\alpha(1 - (d-1)^\alpha) + (d-2)(d^\alpha - (d-1)^\alpha). \end{aligned}$$

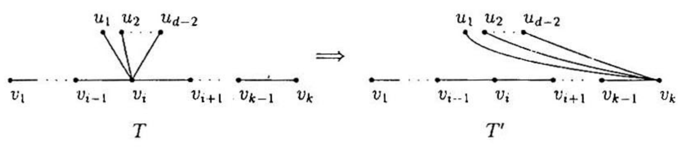

Figure 2.2

If $d \geq 4$, then

$$\begin{aligned} R_\alpha(T) - R_\alpha(T') &> 2^{\alpha+1}(d^\alpha - 2^\alpha) + 2^\alpha(1 - (d-1)^\alpha) \\ &= 2^\alpha(d^\alpha - (d-1)^\alpha + d^\alpha - 2 \cdot 2^\alpha + 1) \\ &> 2^\alpha(4^\alpha - 2 \cdot 2^\alpha + 1) = 2^\alpha(2^\alpha - 1)^2 \geq 0. \end{aligned}$$

Otherwise, $d = 3$ and then

$$\begin{aligned} R_\alpha(T) - R_\alpha(T') &= 2^{\alpha+1}(3^\alpha - 2^\alpha) + 2^\alpha(1 - 2^\alpha) + (3^\alpha - 2^\alpha) \\ &= (6^\alpha + 3^\alpha - 2 \cdot 4^\alpha) + (6^\alpha - 4^\alpha) \\ &> 6^\alpha + 3^\alpha - 2 \cdot 4^\alpha \\ &\geq 2\sqrt{18^\alpha} - 2\sqrt{16^\alpha} > 0. \end{aligned}$$

Therefore, in both cases we get a tree T' with smaller value of the index, which contradicts to the choice of T, and the proof is complete. ∎

3 The cases for $\alpha < 0$

At first we show a lemma which will be used for the proof of the theorem in this section.

Lemma 1 *For $0 < m \leq 1$, if $d, p > 1$, then $g(d,p) = (d+p-1)^{m+1} - (d-1)d^m - (p-1)p^m - d^m p^m > 0$.*

Proof. Since

$$\frac{\partial g}{\partial d} = (m+1)(d+p-1)^m - (m+1)d^m + md^{m-1} - md^{m-1}p^m,$$

we have

$$\begin{aligned} \frac{\partial \frac{\partial g}{\partial d}}{\partial p} &= (m+1)m(d+p-1)^{m-1} - m^2 d^{m-1}p^{m-1} \\ &> m^2((d+p-1)^{m-1} - (dp)^{m-1}). \end{aligned}$$

Since $d, p > 1$, $d + p - 1 < dp$, we have $\frac{\partial \frac{\partial g}{\partial d}}{\partial p} > 0$. Furthermore, $\frac{\partial g}{\partial d}(d, 1) = (m + 1)d^m - (m+1)d^m + md^{m-1} - md^{m-1} = 0$. Só we get $\frac{\partial g}{\partial d} > 0$, for $p > 1$. Since $g(1, p) = p^{m+1} - (p-1)p^m - p^m = 0$, we have $g(d, p) > 0$ for $d, p > 1$. ∎

Theorem 3.1 *Among trees with n vertices, the star S_n has the minimum general Randić index, for $\alpha < 0$.*

Proof. We distinguish the following two cases.

Case 1. $-1 \leq \alpha < 0$.

Assume that a tree T is not a star, but which has the minimum index, for $-1 \leq \alpha < 0$. Let u be the vertex of T with the maximum degree, and so $d(u) < n - 1$. Choose a vertex v with largest degree among all the neighbors of u. Suppose $d(u) = d$ and $d(v) = p$. Then we have $d \geq p \geq 2$. By contracting the edge uv and adding a new leaf edge uw on the new vertex w, we get a new tree T' (see Figure 3.1). Denote by S_u

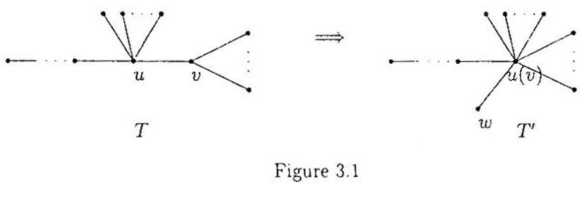

Figure 3.1

the sum of the weights of the edges, other than uv, incident with the vertex u, and S_v

the sum of the weights of the edges, other than uv, incident with the vertex v. Thus we have

$$S_u \geq (d-1)d^\alpha p^\alpha \quad and \quad S_v \geq (p-1)d^\alpha p^\alpha.$$

So,

$$\begin{aligned}
& R_\alpha(T) - R_\alpha(T') \\
= \;& S_u(1 - \frac{(d+p-1)^\alpha}{d^\alpha}) + S_v(1 - \frac{(d+p-1)^\alpha}{p^\alpha}) + (dp)^\alpha - (d+p-1)^\alpha \\
\geq \;& (d-1)p^\alpha(d^\alpha - (d+p-1)^\alpha) + (p-1)d^\alpha(p^\alpha - (d+p-1)^\alpha) + (dp)^\alpha \\
& -(d+p-1)^\alpha \\
= \;& p^\alpha d^\alpha(d+p-1) - (d+p-1)^\alpha((d-1)p^\alpha + (p-1)d^\alpha + 1) \\
= \;& p^\alpha d^\alpha(d+p-1)^\alpha((d+p-1)^{1-\alpha} - (d-1)d^{-\alpha} - (p-1)p^{-\alpha} - d^{-\alpha}p^{-\alpha}) \\
> \;& 0.
\end{aligned}$$

In fact, from Lemma 1, we can easily see that the last inequality holds. Therefore, the new tree T' has a smaller value of index than T, a contradiction.

Case 2. $\alpha < -1$.

Assume that a tree T is not a star for which $R_\alpha(T)$ is minimum for $\alpha < -1$. Let $P = v_0 v_1 \cdots v_{k-1} v_k$ be a longest path of T, such that the degree of v_{k-1} is as large as possible. Note that all the vertices adjacent with v_{k-1} except v_{k-2} are leaves. By deleting all the leaf edges incident with v_{k-1} and connecting each of these leaf vertices to the vertex v_{k-2} by new edges, we get a new tree T', as shown in Figure 3.2. Now

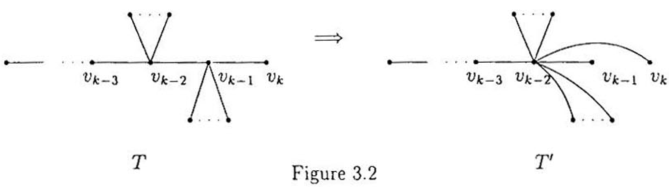

Figure 3.2

we will show that the value of general Randić index of T' is smaller than that of T, and thus lead to a contradiction. Suppose $d(v_{k-1}) = p \geq 2$, $d(v_{k-2}) = d \geq 2$ and $d(v_{k-3}) = t$. We denote by S_d the sum of the weights of all the edges incident with v_{k-2}, except $v_{k-2}v_{k-1}$.

Let w be the neighbor of v_{k-2}, other than v_{k-1} and v_{k-3}. Then $d(w) \leq p$. Since $S_d \geq (d-2)d^\alpha p^\alpha + d^\alpha t^\alpha$, we have

$$\begin{aligned}
& R_\alpha(T) - R_\alpha(T') \\
= \;& S_d\left(1 - \frac{(d+p-1)^\alpha}{d^\alpha}\right) + (dp)^\alpha + (p-1)p^\alpha - p(d+p-1)^\alpha \\
\geq \;& ((d-2)p^\alpha + t^\alpha)(d^\alpha - (d+p-1)^\alpha) + (dp)^\alpha + (p-1)p^\alpha - p(d+p-1)^\alpha \\
> \;& (d-2)p^\alpha(d^\alpha - (d+p-1)^\alpha) + (dp)^\alpha + (p-1)p^\alpha - p(d+p-1)^\alpha \\
= \;& (d-1)p^\alpha d^\alpha - (d-2)p^\alpha(d+p-1)^\alpha - p(d+p-1)^\alpha + (p-1)p^\alpha \\
= \;& p^\alpha d^\alpha (p+d-1)^\alpha((d-1)(p+d-1)^{-\alpha} - (d-2)d^{-\alpha} \\
& -p \cdot p^{-\alpha} d^{-\alpha} + (p-1)d^{-\alpha}(p+d-1)^{-\alpha}).
\end{aligned}$$

In order to show $R_\alpha(T) > R_\alpha(T')$, it is sufficient to show that

$$f(d,p) = (d-1)(p+d-1)^{-\alpha} - (d-2)d^{-\alpha} - p \cdot p^{-\alpha}d^{-\alpha} + (p-1)d^{-\alpha}(p+d-1)^{-\alpha} > 0.$$

Let $\beta = -\alpha > 1$. Since

$$(d-1)(p+d-1)^\beta - (d-2)d^\beta = (d-1)((p+d-1)^\beta - d^\beta) + d^\beta > d^\beta,$$

we have

$$\begin{aligned}
f(d,p) \;&>\; d^\beta - p^{\beta+1}d^\beta + (p-1)d^\beta(p+d-1)^\beta \\
&=\; d^\beta(1 - p^{\beta+1} + (p-1)(p+d-1)^\beta) \\
&\geq\; d^\beta((p-1)(p+1)^\beta - p^{\beta+1} + 1) \\
&=\; d^\beta((p-1)((p+1)^\beta - p^\beta) - (p^\beta - 1)) \\
&=\; d^\beta((p-1)\beta\xi^{\beta-1} - \beta\eta^{\beta-1}(p-1)) \\
&=\; d^\beta\beta(p-1)(\xi^{\beta-1} - \eta^{\beta-1})
\end{aligned}$$

where $p \leq \xi \leq p+1$, $1 \leq \eta \leq p$ and $\beta > 1$. So we have $\xi^{\beta-1} - \eta^{\beta-1} \geq 0$, that is $R_\alpha(T) - R_\alpha(T') > 0$. This completes the proof. ∎

4 Conclusion

In this paper we obtain the trees with the minimum value of the general Randić index. It turns out that for α in different intervals this extremal tree is unique, and only two intervals are distinguished. In order to give a clear picture, we use the following table to summarize our main results.

α	$\alpha < 0$	$\alpha > 0$
extremal tree	star	path ($n \geq 5$)
minimum value	$(n-1)^{\alpha+1}$	$2^{\alpha+1} + (n-3)4^{\alpha}$ ($n \geq 5$)

In another successive paper we shall discuss trees with maximum value of general Randić index. The discussion becomes much more complicated.

References

[1] B. Bollobás and P. Erdős, Graphs of extremal weights, Ars Combin. 50(1998) 225-233.

[2] B. Bollobás, P. Erdős and A. Sakar, Extremal graphs for weights, Discrete Math. 200(1999) 5-19.

[3] J.A. Bondy and U.S.R. Murty, Graph Theory With Applications, Macmllan Press Ltd. London, 1976.

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

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

[6] C. Delorme, O. Favaron and D. Rautenbach, On the Randić index, Discr. Math. 257(2002) 29-38.

[7] X. Li and Y.T. Yang, Sharp bounds for the general Randić index, Accepted for publication in MATCH Commun. Math. Compt. Chem. 2003.

[8] M. Randić, On characterization of molecular branching, J. Am. Chem. Soc. 97(1975) 6609-6615.

[9] N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, 1992.

[10] P. Yu, An upper bound for the Randić indices of trees, J. Math. Study (Chinese) 31(1998) 225-230.