Trees with a given order and matching number that have maximum general Randić index *

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Abstract

The general Randić index $R_\alpha(G)$ of a graph G is defined by $R_\alpha(G) = \sum_{uv}(d(u)d(v))^\alpha$, where $d(u)$ is the degree of a vertex u, and the summation extends over all edges uv of G. Some results on trees with a given order and matching number that have minimum general Randić index have been obtained. However, the corresponding maximum problem has not been studied, and usually the maximum problem is much harder than the minimum one. In this paper, we characterize the structure of the trees with a given order and matching number that have maximum general Randić index for $\alpha > 1$ and give sharp upper bound for $0 < \alpha \leq 1$.

Key words: general Randić index, tree, matching

AMS Subject Classification: 05C35, 92E10, 05C05

1 Introduction

The general Randić index $R_\alpha(G)$ of a graph G is defined by

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

where $d(u)$ is the degree of a vertex u in G and the summation extends over all edges uv of G. It is known that the index $R_{-\frac{1}{2}}$ was introduced by Randić [16] in 1975 as a topological index, suitable for measuring the extent of branching of the carbon-atom skeleton of saturated hydrocarbons. Randić himself demonstrated [16] that his index, i.e., the Randić index, is well correlated with a variety of physico-chemical properties of alkanes. $R_{-\frac{1}{2}}$ becomes one of the most popular molecular descriptors to which at least three books are devoted [7, 8, 9]. In 1998, Bollobás and Erdős [1]

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generalized this index by replacing $-\frac{1}{2}$ by any real number α, which is called the general Randić index.

The problems of finding the upper or lower bounds for the general Randić index and finding the corresponding extremal graphs have attracted much attention of many researchers (see the surveys [10, 11]). For examples, Yu [17] showed that $R_{-\frac{1}{2}}(T) \leq \frac{n+2\sqrt{2}-3}{2}$ for any tree T of order n. Later, Gaporossi et al. [3] obtained the same result by using an alternative approach. Clark and Moon [4] showed that $1 \leq R_{-1}(T) \leq \frac{5n+8}{18}$ and proposed two unsolved questions on the upper bound. These two questions were positively answered in [6, 14, 15].

In [12], Lu et al. established a sharp lower bound of $R_{-\frac{1}{2}}$ for conjugated trees (trees with a Kekulé structure or, equivalently, trees with a perfect matching) as well as the trees with a given size of maximum matchings, called *matching number*. Pan et al. [13] generalized this result by extending the number $\alpha = -\frac{1}{2}$ to $\alpha \in [-\frac{1}{2}, 0)$. They also gave a sharp lower bound of R_α for the trees with a given matching number for $\alpha > 0$. Recently, Chen et al. [5] gave a sharp lower bound of R_α for conjugated trees for $\alpha \leq -1$. As one can see in [4, 6, 14, 15], usually the maximum problem is much harder than the minimum one. In this paper, we characterize the structure of trees with the maximum value of R_α for $\alpha > 1$ with a prescribed order and matching number (see Corollary 3.1) and a sharp upper bound for $0 < \alpha \leq 1$ as well as the corresponding extremal tree (see Theorem 3.4).

For convenience, we first introduce some terminology and notations. All graphs considered in the following will be simple. The set of vertices and the set of edges of a graph G is denoted by $V(G)$ and $E(G)$, respectively. The *order* of G is defined by $|V(G)|$ and the *size* of G is defined by $|E(G)|$. The *degree* $d_G(u)$ of a vertex u of G is the number of vertices adjacent to u in G. A vertex of degree one is called *pendent vertex*. We use Δ to denotes the *maximum degree* of G. The *neighborhood* of u is denoted by $N(u)$. The *length* of a path P is the number of edges of it and denoted by $|P|$. A path $P = v_0v_1\cdots v_l$ is called a *pendent path* if $d(v_0) \geq 3,\ d(v_l) = 1$ and $d(v_1) = \cdots = d(v_{l-1}) = 2$. A path $P = v_0v_1\cdots v_k$ is called an *internal path* if $d(v_0) \geq 3,\ d(v_k) \geq 3$ and $d(v_1) = \cdots = d(v_{k-1}) = 2$. Undefined terminology and notations can be found in [2].

2 Properties of an extremal tree

Let $\mathcal{T}_{n,m}(n \geq 2m)$ be the set of trees of order n with a given matching number m and $\mathbf{M}(T)$ be a maximum matching of T. In the following we always assume that the tree $T^* \in \mathcal{T}_{n,m}$ has the maximum general Randić index for $\alpha > 0$. And let $\mathbf{M}^*$ be a fixed maximum matching of T^*, which means, for any $T \in \mathcal{T}_{n,m}$, $R_\alpha(T^*) \geq R_\alpha(T)$ $(\alpha > 0)$.

Obviously, for $m = 1$ or $m = 2, n \leq 4$ we have

Theorem 2.1 *If $m = 1$, then T^* is the star S_n. If $m = 2$ and $n = 4$, then T^* is the path P_4.*

From Theorem 2.1, we can just consider the case for $m \geq 2$ and $n \geq 5$ in the following discussion.

Lemma 2.2 *For $\alpha > 0$, if $T^* \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$, then T^* is not a path, i.e. $\Delta(T^*) \geq 3$.*

Proof. Suppose the assertion of the lemma is false, let $T^* = v_0v_1 \cdots v_{n-1}$ be a path. Let $T' = T^* + \{v_1v_3\} - \{v_1v_2\}$, then $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$. If $n = 5$, $R_\alpha(T') - R_\alpha(T^*) = (2^\alpha + 2 \cdot 3^\alpha + 6^\alpha) - (2 \cdot 2^\alpha + 2 \cdot 4^\alpha) > (6^\alpha - 4^\alpha) - (4^\alpha - 3^\alpha) > 0$. For $n \geq 6$, $R_\alpha(T') - R_\alpha(T^*) = 2^\alpha + 3^\alpha + 2 \cdot 6^\alpha - 2^\alpha - 3 \cdot 4^\alpha = 2(6^\alpha - 4^\alpha) - (4^\alpha - 3^\alpha) > (6^\alpha - 4^\alpha) - (4^\alpha - 3^\alpha) > 0$. This is because, by the Lagrange mean-value theorem, we have $(6^\alpha - 4^\alpha) - (4^\alpha - 3^\alpha) = \alpha(2\xi_1^{\alpha-1} - \xi_2^{\alpha-1})$, where $\xi_1 \in (4, 6), \xi_2 \in (3, 4)$. It is obvious that $\alpha(2\xi_1^{\alpha-1} - \xi_2^{\alpha-1}) > 0$ for $\alpha \geq 1$. For $\alpha \in (0, 1)$, $\alpha(2\xi_1^{\alpha-1} - \xi_2^{\alpha-1}) > \alpha(2 \cdot 6^{\alpha-1} - 3^{\alpha-1}) > 0$, since $(\frac{6}{3})^{1-\alpha} = 2^{1-\alpha} < 2$. Therefore, we deduce a contradiction and finish the proof. ∎

Lemma 2.3 *Let P be a pendent path of $T^* \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$, then $|P| \leq 2$.*

Proof. Assume to the contrary that $P = v_0v_1 \cdots v_l (l \geq 3)$ is a pendent path of T^* with $d(v_0) = t \geq 3$, $d(v_l) = 1$, $d(v_1) = \cdots = d(v_{l-1}) = 2$ and $|P| = l \geq 3$. Denote $N_0 = N_{T^*}(v_0) \setminus \{v_1\}$. Let $T' = T^* - \{v_{l-2}v_{l-1}\} + \{v_0v_l\}$, we have $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$.

If $l \geq 4$, then

$$\begin{aligned}
&R_\alpha(T') - R_\alpha(T^*) \\
=&[(t+1)^\alpha - t^\alpha]\left(\sum_{u \in N_0} d(u)^\alpha + 2^\alpha\right) + 2^\alpha[(t+1)^\alpha - 2^{\alpha+1} + 1] \\
>&2^\alpha[(t+1)^\alpha - 2^{\alpha+1} + 1] > 2^\alpha(4^\alpha - 2^{\alpha+1} + 1) = 2^\alpha(2^\alpha - 1)^2 > 0,
\end{aligned}$$

since $(t+1)^\alpha - 2^{\alpha+1} + 1$ is monotonically increasing in $t \geq 3$.

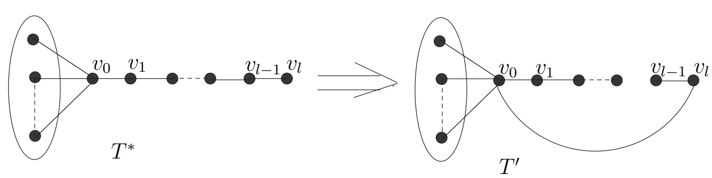

Figure 2.1 T^* and T' in Lemma 2.3.

If $l = 3$, $R_\alpha(T') - R_\alpha(T^*) = [(t+1)^\alpha - t^\alpha]\left(\sum_{u \in N_0} d(u)^\alpha + 2^\alpha\right) + [(t+1)^\alpha - 4^\alpha] > 0$.

This is a contradiction to the assumption of T^*, and so $l \leq 2$. ∎

Lemma 2.4 *For $\alpha > 0$, if P is an internal path of $T^* \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$, then $|P| \leq 1$.*

Proof. Suppose to the contrary that $P = v_0v_1 \cdots v_k (k \geq 2)$ is an internal path of T^* with $d(v_0) = t \geq 3$, $d(v_k) = s \geq 3$, $d(v_1) = \cdots = d(v_{k-1}) = 2$ and $|P| = k \geq 2$.

Let $N_0 = N_{T^*}(v_0) \setminus \{v_1\}$ and $N_1 = N_{T^*}(v_k) \setminus \{v_{k-1}\}$.

Case 1. $k \geq 5$.

Let $T' = T^* - \{v_1v_2, v_3v_4\} + \{v_0v_2, v_1v_4\}$, we have $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$. Then $R_\alpha(T') - R_\alpha(T^*) = [(t+1)^\alpha - t^\alpha]\left(\sum_{u \in N_0} d(u)^\alpha + 2^\alpha\right) + 2^\alpha[(t+1)^\alpha - 2^{\alpha+1} + 1] > 0$, a contradiction.

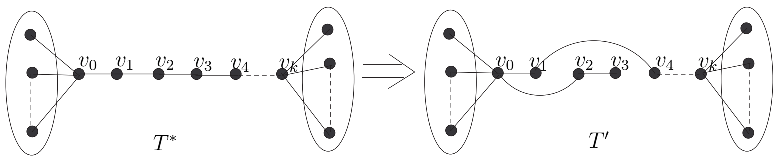

Figure 2.2 T^* and T' of Case 1 in Lemma 2.4.

Case 2. $k = 4$.

Subcase 2.1. v_2 is $\mathbf{M}^*$-unsaturated.

Then v_1 and v_3 must be $\mathbf{M}^*$-saturated. Let $T' = T^* + \{v_0v_2, v_1v_3\} - \{v_1v_2, v_2v_3\}$, then $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$ and $R_\alpha(T') - R_\alpha(T^*) = [(t+1)^\alpha - t^\alpha]\left(\sum_{u \in N_0} d(u)^\alpha + 2^\alpha\right) + (t+1)^\alpha - 4^\alpha > 0$, a contradiction.

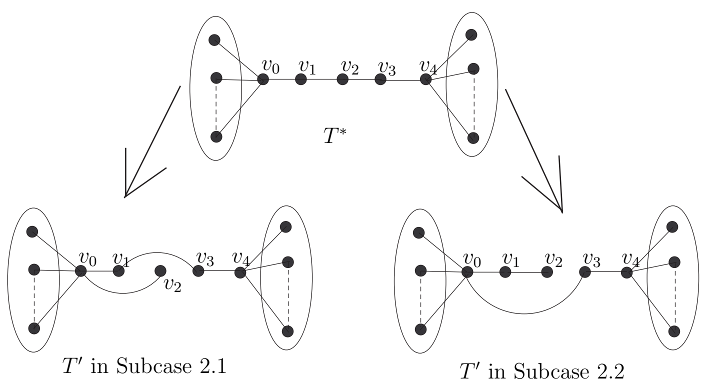

Figure 2.3 T^* and T' of Case 2 in Lemma 2.4.

Subcase 2.2. v_2 is $\mathbf{M}^*$-saturated, and we may let $v_1v_2 \in \mathbf{M}^*$.

Then, at least one vertex of $\{v_0, v_3\}$ is $\mathbf{M}^*$-saturated. Let $T' = T^* + \{v_0v_3\} - \{v_2v_3\}$ and we have $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$. Then

$$\begin{aligned}
&R_\alpha(T') - R_\alpha(T^*) \\
=&[(t+1)^\alpha - t^\alpha]\left(\sum_{u\in N_0} d(u)^\alpha + 2^\alpha\right) + 2^\alpha[(t+1)^\alpha - 2^{\alpha+1} + 1)] \\
>&2^\alpha[(t+1)^\alpha - 2^\alpha - (2^\alpha - 1)] \geq 2^\alpha[(4^\alpha - 2^\alpha) - (2^\alpha - 1)] \\
=&2^\alpha(2^\alpha - 1)^2 > 0,
\end{aligned}$$

a contradiction.

Case 3. $k = 3$.

Subcase 3.1. $v_1v_2 \in \mathbf{M}^*$.

Let $T' = T^* - \{v_2v_3\} + \{v_0v_3\}$, we have $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$. Then

$$\begin{aligned}
&R_\alpha(T') - R_\alpha(T^*) \\
=&[(t+1)^\alpha - t^\alpha]\left(\sum_{u\in N_0} d(u)^\alpha + 2^\alpha\right) + (t+1)^\alpha s^\alpha + 2^\alpha - 4^\alpha - (2s)^\alpha \\
>&(t+1)^\alpha s^\alpha + 2^\alpha - 4^\alpha - (2s)^\alpha > (4s)^\alpha + 2^\alpha - 4^\alpha - (2s)^\alpha \\
=&2^\alpha(2^\alpha - 1)(s^\alpha - 1) > 0,
\end{aligned}$$

a contradiction.

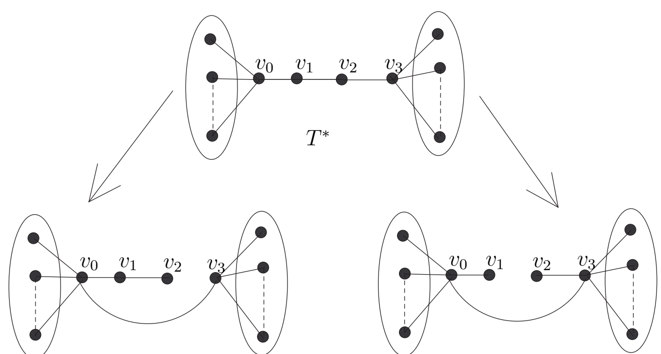

Figure 2.4 T^* and T' of Case 3 in Lemma 2.4.

Subcase 3.2. $v_1v_2 \notin \mathbf{M}^*$.

Let $T' = T^* - \{v_1v_2\} + \{v_0v_3\}$, we have $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$. Then

$$\begin{aligned}
R_\alpha(T') - R_\alpha(T^*) =&[(t+1)^\alpha - t^\alpha]\sum_{u\in N_0} d(u)^\alpha + [(s+1)^\alpha - s^\alpha]\sum_{w\in N_1} d(w)^\alpha \\
&+ (t+1)^\alpha(s+1)^\alpha + (t+1)^\alpha + (s+1)^\alpha - (2t)^\alpha - (2s)^\alpha - 4^\alpha.
\end{aligned}$$

Let $F_1(s,t) := (t+1)^\alpha(s+1)^\alpha + (t+1)^\alpha + (s+1)^\alpha - (2t)^\alpha - (2s)^\alpha - 4^\alpha$, then

$$\frac{\partial F_1(s,t)}{\partial s} = \alpha[(t+1)^\alpha(s+1)^{\alpha-1} + (s+1)^{\alpha-1} - 2^\alpha s^{\alpha-1}].$$

If $\alpha \geq 1$, then $(t+1)^\alpha > 2^\alpha$, which implies $\frac{(t+1)^\alpha+1}{2^\alpha} > 1 \geq \left(\frac{s}{s+1}\right)^{\alpha-1}$.

If $\alpha \in (0,1)$, then $\frac{(t+1)^\alpha+1}{2^\alpha} = \left(\frac{t+1}{2}\right)^\alpha + \frac{1}{2^\alpha} > 1 + \frac{1}{2} > 1 + \frac{1}{s} > \left(\frac{s}{s+1}\right)^{\alpha-1}$.
Therefore, $\frac{(t+1)^\alpha+1}{2^\alpha} > \left(\frac{s}{s+1}\right)^{\alpha-1}$, for $\alpha > 0$. Thus $\frac{\partial F_1(s,t)}{\partial s} > 0$.

Similarly, we have $\frac{\partial F_1(s,t)}{\partial t} > 0$. Thereby, $F_1(s,t) \geq F_1(3,3) = 16^\alpha - 2\times 8^\alpha + 4^\alpha = 4^\alpha(2^\alpha-1)^2 > 0$. Consequently, we have $R(T') > R(T^*)$, a contradiction.

Case 4. $k = 2$.

Subcase 4.1. v_1 is $\mathbf{M}^*$-unsaturated.

Then, v_0 and v_2 are both $\mathbf{M}^*$-saturated. Let $T' = T^* + \{v_0v_2\} - \{v_1v_2\}$, then $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$ and $\mathbf{M}^*$ is also a maximum matching of T'.

$$R_\alpha(T') - R_\alpha(T^*) = [(t+1)^\alpha - t^\alpha]\sum_{u\in N_0} d(u)^\alpha + (t+1)^\alpha(s^\alpha+1) - 2^\alpha(s^\alpha+t^\alpha).$$

Let $F_2(s,t) := (t+1)^\alpha(s^\alpha+1) - 2^\alpha(s^\alpha+t^\alpha)$, then $\frac{\partial F_2(s,t)}{\partial s} = \alpha s^{\alpha-1}[(t+1)^\alpha - 2^\alpha] > 0$. If $\alpha \geq 1$, then $s^\alpha + 1 > 2^\alpha$, which implies $\frac{s^\alpha+1}{2^\alpha} > 1 \geq \left(\frac{t}{t+1}\right)^{\alpha-1}$,
else if $\alpha \in (0,1)$, $\frac{s^\alpha+1}{2^\alpha} = \left(\frac{s}{2}\right)^\alpha + \frac{1}{2^\alpha} > 1 + \frac{1}{2} > 1 + \frac{1}{3} \geq 1 + \frac{1}{t} = \frac{t+1}{t} > \left(\frac{t}{t+1}\right)^{\alpha-1}$.

Hence $\frac{\partial F_2(s,t)}{\partial t} = \alpha[(t+1)^{\alpha-1}(s^\alpha+1) - 2^\alpha t^{\alpha-1}] > 0, \quad \text{for} \quad \alpha > 0$. Therefore

$$\begin{aligned} F_2(s,t) \geq& F_2(3,3) = (12^\alpha - 6^\alpha) - (6^\alpha - 4^\alpha) \\ >& (12^\alpha - 8^\alpha) - (6^\alpha - 4^\alpha) = 2^\alpha(2^\alpha-1)(3^\alpha-2^\alpha) > 0. \end{aligned}$$

Consequently, we have $R(T') > R(T^*)$, a contradiction.

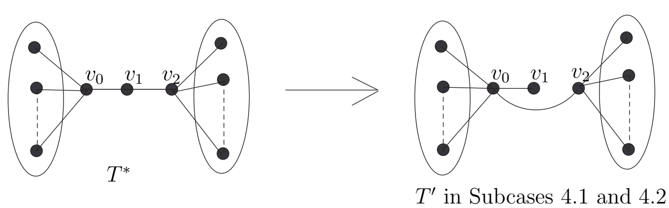

Figure 2.5 T^* and T' of Case 4 in Lemma 2.4.

Subcase 4.2. v_1 is $\mathbf{M}^*$-saturated, and we may let $v_0v_1 \in M^*$.

We can use the same transformation in Subcase 4.1, and we also get a contradiction to the assumption of T^*. ∎

Lemma 2.5 *Let $V^* = \{v \in T^*, d(v) \geq 3\}$, then $|V^*| \leq 2$ for $\alpha > 0$.*

Proof. Assume, to the contrary, $|V^*| \geq 3$, then by Lemma 2.4, there exist $v_0, v_1, v_2 \in V^*$, such that $v_0v_1, v_1v_2 \in E(T^*)$. Let $d(v_0) = t, d(v_1) = s, d(v_2) = r$.

Case 1. Only one vertex of $\{v_0, v_1, v_2\}$ is $\mathbf{M}^*$-saturated.

Then it must be vertex v_1. Define $N_0 = N_{T^*}(v_0) \setminus \{v_1\}$, $N_1 = N_{T^*}(v_1) \setminus \{v_0, v_2\}$ and $N_2 = N_{T^*}(v_2) \setminus \{v_1\}$, respectively. Then every vertex in N_0 and N_2 are $\mathbf{M}^*$-saturated. If $\alpha \geq 1$, let $T' =$

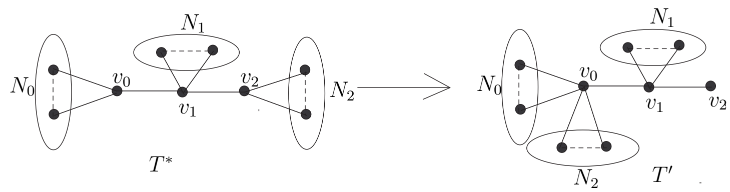

Figure 2.6 T^* and T' of Case 1 and 2 for $\alpha \geq 1$ in Lemma 2.5.

$T^* - \bigcup_{v \in N_2} \{v_2v\} + \bigcup_{v \in N_2} \{v_0v\}$, then $\mathbf{M}^*$ is a maximum matching of T', so $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$ and

$$\begin{aligned}
&R_\alpha(T') - R_\alpha(T^*) \\
=&(t+r-1)^\alpha \left(\sum_{u \in N_0} d(u)^\alpha + \sum_{w \in N_2} d(w)^\alpha \right) + s^\alpha + (t+r-1)^\alpha s^\alpha \\
&- (st)^\alpha - (sr)^\alpha - t^\alpha \sum_{u \in N_0} d(u)^\alpha - r^\alpha \sum_{w \in N_2} d(w)^\alpha \\
>&s^\alpha[1 + (t+r-1)^\alpha - t^\alpha - r^\alpha] \geq 0.
\end{aligned}$$

If $0 < \alpha < 1$, let $T' = T^* - \bigcup_{v \in N_2} \{v_2v\} + \bigcup_{v \in N_2} \{v_1v\}$, then $\mathbf{M}^*$ is a maximum matching of T', so $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$ and

$$\begin{aligned}
&R_\alpha(T') - R_\alpha(T^*) \\
=&\sum_{u \in N_2} d(u)^\alpha[(s+r-1)^\alpha - r^\alpha] + \sum_{w \in N_1} d(w)^\alpha[(s+r-1)^\alpha - s^\alpha] \\
&+ (s+r-1)^\alpha - s^\alpha r^\alpha + t^\alpha(s+r-1)^\alpha - t^\alpha s^\alpha.
\end{aligned}$$

By the Lagrange mean-value theorem, there exist $a \in (r, s+r-1)$, $b \in (s, s+r-1)$ and $c \in (s+r-1, sr)$, such that $(s+r-1)^\alpha - r^\alpha = \alpha(s-1)a^{\alpha-1}$, $(s+r-1)^\alpha - s^\alpha = \alpha(r-1)b^{\alpha-1}$

and $(sr)^\alpha - (s+r-1)^\alpha = \alpha(s-1)(r-1)c^{\alpha-1}$. Hence we have

$$
\begin{aligned}
&R_\alpha(T') - R_\alpha(T^*)\\
\geq&(r-1)[(s+r-1)^\alpha - r^\alpha] + (s-1)[(s+r-1)^\alpha - s^\alpha] + (s+r-1)^\alpha - s^\alpha r^\alpha\\
=&\alpha(r-1)(s-1)a^{\alpha-1} + \alpha(s-1)(r-1)b^{\alpha-1} - \alpha(s-1)(r-1)c^{\alpha-1}\\
=&\alpha(s-1)(r-1)[a^{\alpha-1} + b^{\alpha-1} - c^{\alpha-1}] > 0,
\end{aligned}
$$

since $x^{\alpha-1}$ is monotonically decreasing in $x \geq 3$ for $0 < \alpha < 1$, and $a < c,\ b < c$.

Case 2. Exactly two vertices of $\{v_0, v_1, v_2\}$ are $\mathbf{M}^*$-saturated.

Subcase 2.1. v_0, v_2 are $\mathbf{M}^*$-saturated. Assume $v_2x \in \mathbf{M}^*$.

If $\alpha \geq 1$, let $T' = T^* - \bigcup\limits_{v\in N_2}\{v_2v\} + \bigcup\limits_{v\in N_2}\{v_0v\}$.

If $0 < \alpha < 1$, let $T' = T^* - \bigcup\limits_{v\in N_2}\{v_2v\} + \bigcup\limits_{v\in N_2}\{v_1v\}$.

Then $\mathbf{M}^* - \{v_2x\} + \{v_1v_2\}$ is a maximum matching of T', that is $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$. And Similar to Case 1, we then deduce a contradiction.

Subcase 2.2. v_0, v_1 are $\mathbf{M}^*$-saturated. With the same transformation in Subcase 2.1, then $\mathbf{M}^*$ is a maximum matching of T', we get a contradiction.

Subcase 2.3. v_1, v_2 are $\mathbf{M}^*$-saturated. Assume $v_2x \in \mathbf{M}^*$.

Similar to Case 1, if $\alpha \geq 1$, let $T' = T^* - \bigcup\limits_{v\in N_0}\{v_0v\} + \bigcup\limits_{v\in N_0}\{v_2v\}$; if $0 < \alpha < 1$, let $T' = T^* - \bigcup\limits_{v\in N_0}\{v_0v\} + \bigcup\limits_{v\in N_0}\{v_1v\}$, then $\mathbf{M}^*$ is a maximum matching of T', i.e., $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$. And with the same calculation in Case 1, we have $R(T') > R(T^*)$, a contradiction to the assumption of T^*.

Case 3. $\{v_0, v_1, v_2\}$ are all $\mathbf{M}^*$-saturated.

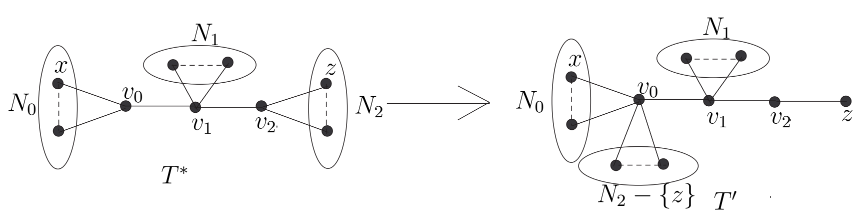

Figure 2.7 T^* and T' of Case 3 for $\alpha \geq 1$ in Lemma 2.5.

Subcase 3.1. $v_0v_1 \in \mathbf{M}^*$ or $v_1v_2 \in \mathbf{M}^*$.

If $\alpha \geq 1$, assume $v_0v_1 \in \mathbf{M}^*$ without loss of generality, then there exists $z \in V(T^*) \setminus \{v_0, v_1\}$ such that $v_2z \in \mathbf{M}^*$. Let $T' = T^* - \bigcup\limits_{v\in N_2}\{v_2v\} + \bigcup\limits_{v\in N_2}\{v_0v\}$, then $\mathbf{M}^* - \{v_0v_1, v_2z\} + \{v_1v_2, v_0z\}$

is a maximum matching of T'. We then deduce a contradiction.

If $0 < \alpha < 1$, assume $v_1v_2 \in \mathbf{M}^*$, let $T' = T^* - \bigcup_{v \in N_0} \{v_0v\} + \bigcup_{v \in N_0} \{v_1v\}$, then $\mathbf{M}^*$ is a maximum matching of T'. We obtain a contradiction by a similar calculation in Case 1.

Subcase 3.2. $v_0v_1, v_1v_2 \notin \mathbf{M}^*$, i.e., $\exists x \in N_0, y \in N_1, z \in N_2$, such that $v_0x, v_1y, v_2z \in \mathbf{M}^*$. That is to say, each vertex in V^* is $\mathbf{M}^*$-saturated.

Next we will show that if $v \in V^*$ and $vu \in \mathbf{M}^*$, then $d(u) = 1$.

Since $v_0x \in \mathbf{M}^*$, if $d(x) \geq 3$, then we choose x, v_0, v_1 instead of v_0, v_1, v_2 for consideration, and back to Subcase 3.1, we get a contradiction.

If $d(x) = 2$, then the degree of the vertex u which adjacent to x other than v_0 is one (by Lemmas 2.3 and 2.4). Obviously, $\mathbf{M}^* - \{v_0x\} + \{ux\}$ is a maximum matching of T^*, too. Meanwhile, there are exactly two vertices of $\{v_0, v_1, v_2\}$ that are saturated by $\mathbf{M}^* - \{v_0x\} + \{ux\}$, then back to Case 2, hence we get a contradiction.

Therefore, $d(x) = 1$. Similarly, $d(y) = 1$ and $d(z) = 1$.

Now assume, without loss of generality, $t \geq r \geq 3$.

If $\alpha \geq 1$, let $T' = T^* - \bigcup_{w \in N_2 \setminus \{z\}} \{v_2w\} + \bigcup_{w \in N_2 \setminus \{z\}} \{v_0w\}$, then we have

$$
\begin{aligned}
&R_\alpha(T') - R_\alpha(T^*) \\
=&(t+r-2)^\alpha \cdot s^\alpha + 2^\alpha \cdot s^\alpha + 2^\alpha - (ts)^\alpha - (sr)^\alpha - r^\alpha \\
&+ [(t+r-2)^\alpha - t^\alpha] \sum_{w_0 \in N_0} d(w_0)^\alpha + [(t+r-2)^\alpha - r^\alpha] \sum_{w_2 \in N_2 \setminus \{z\}} d(w_2)^\alpha \\
>&(t+r-2)^\alpha \cdot s^\alpha + 2^\alpha \cdot s^\alpha + 2^\alpha - (ts)^\alpha - (sr)^\alpha - r^\alpha \\
&+ [(t+r-2)^\alpha - r^\alpha] \sum_{w_2 \in N_2 \setminus \{z\}} d(w_2)^\alpha \\
>&(r-2)[(t+r-2)^\alpha - r^\alpha] - r^\alpha + 2^\alpha + s^\alpha[(t+r-2)^\alpha - t^\alpha - r^\alpha + 2^\alpha] \\
>&[(t+r-2)^\alpha - r^\alpha] - r^\alpha + 2^\alpha \geq [(t^\alpha + r^\alpha - 2^\alpha) - r^\alpha] - r^\alpha + 2^\alpha = t^\alpha - r^\alpha \geq 0,
\end{aligned}
$$

since the function $F_3(t, r) := (t+r-2)^\alpha - t^\alpha - r^\alpha + 2^\alpha$ is monotonically increasing in $t \geq 2$ and $r \geq 2$ for $\alpha \geq 1$, respectively. This is a contradiction.

If $0 < \alpha < 1$, let $T' = T^* - \bigcup_{v \in N_0 \setminus \{x\}} \{v_0v\} + \bigcup_{v \in N_0 \setminus \{x\}} \{v_1v\}$, then $\mathbf{M}^*$ is a maximum matching of T' and

$$\begin{aligned}
&R_\alpha(T') - R_\alpha(T^*)\\
=&[(t+s-2)^\alpha - t^\alpha] \sum_{v\in N_0\setminus\{x\}} d(v)^\alpha + 2^\alpha - t^\alpha + 2^\alpha(t+s-2)^\alpha\\
&+ [(t+s-2)^\alpha - s^\alpha] \sum_{v\in N_1} d(v)^\alpha + r^\alpha(t+s-2)^\alpha - s^\alpha(r^\alpha + t^\alpha)\\
\geq&(t-2)[(t+s-2)^\alpha - t^\alpha] + 2^\alpha - t^\alpha + 2^\alpha(t+s-2)^\alpha - t^\alpha s^\alpha\\
&+ (s-2)[(t+s-2)^\alpha - s^\alpha] + r^\alpha(t+s-2)^\alpha - s^\alpha r^\alpha.
\end{aligned}$$

Let $F_4(t,s,r) := (t-2)[(t+s-2)^\alpha - t^\alpha] + 2^\alpha - t^\alpha + 2^\alpha(t+s-2)^\alpha - t^\alpha s^\alpha + (s-2)[(t+s-2)^\alpha - s^\alpha] + r^\alpha(t+s-2)^\alpha - s^\alpha r^\alpha$. Since $\frac{\partial F_4(t,s,r)}{\partial r} = \alpha r^{\alpha-1}[(t+s-2)^\alpha - s^\alpha] > 0$, we have

$$\begin{aligned}
F_4(t,s,r) > F_4(t,s,1) =&(t-2)[(t+s-2)^\alpha - t^\alpha] + (s-1)[(t+s-2)^\alpha - s^\alpha]\\
&- (t^\alpha - 2^\alpha) - [t^\alpha s^\alpha - 2^\alpha(t+s-2)^\alpha].
\end{aligned}$$

By the Lagrange mean-value theorem, there exist $a \in (t, t+s-2)$, $b \in (s, t+s-2)$, $c \in (2,t)$ and $d \in (2t+2s-4, ts)$, such that $(t+s-2)^\alpha - t^\alpha = \alpha(s-2)a^{\alpha-1}$, $(t+s-2)^\alpha - s^\alpha = \alpha(t-2)b^{\alpha-1}$, $t^\alpha - 2^\alpha = \alpha(t-2)c^{\alpha-1}$, and $(ts)^\alpha - (2t+2s-4)^\alpha = \alpha(t-2)(s-2)d^{\alpha-1}$. Hence we have

$$\begin{aligned}
F_4(t,s,r) >&\alpha(s-2)(t-2)a^{\alpha-1} + \alpha(s-1)(t-2)b^{\alpha-1} - \alpha(t-2)c^{\alpha-1}\\
&- \alpha(s-2)(t-2)d^{\alpha-1}\\
=&\alpha(t-2)[(s-2)a^{\alpha-1} + (s-1)b^{\alpha-1} - (s-2)d^{\alpha-1} - c^{\alpha-1}]\\
\geq&\alpha(t-2)[(s-2)(t+s-2)^{\alpha-1} + (s-1)(t+s-2)^{\alpha-1}\\
&- (s-2)(2s+2t-4)^{\alpha-1} - 2^{\alpha-1}]\\
>&\alpha(t-2)[(s-1)(t+s-2)^{\alpha-1} - 2^{\alpha-1}].
\end{aligned}$$

Define $F_5(t,s) := \alpha(t-2)[(s-1)(t+s-2)^{\alpha-1} - 2^{\alpha-1}]$. If $s \geq t$, then $F_5(t,s) \geq \alpha(t-2)[(s-1)(2s-2)^{\alpha-1} - 2^{\alpha-1}] = \alpha(t-2)2^{\alpha-1}[(s-1)^\alpha - 1] > 0$. If $s \leq t$, then $F_5(t,s) \geq \alpha(t-2)[(t-1)(2t-2)^{\alpha-1} - 2^{\alpha-1}] = \alpha(t-2)2^{\alpha-1}[(t-1)^\alpha - 1] > 0$. Therefore $R_\alpha(T') - R_\alpha(T^*) > 0$, a contradiction. Therefore, Lemma 2.5 is proved. ∎

3 Analyzing the structure of an extremal tree

From Lemma 2.2 to Lemma 2.5, obviously we get a rough structure of T^*:

Corollary 3.1 *For $T^* \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$,*

(1) If $|V^*| = 1$, assume $V^* = \{w\}$, then the attached parts of w are either pendent paths of length

1 or pendent paths of length 2;

(2) If $|V^*| = 2$, assume $V^* = \{u, v\}$, then $uv \in E(T^*)$. Besides u and v, the attached parts of u and v are either pendent paths of length 1 or pendent paths of length 2. (See Figure 3.1)

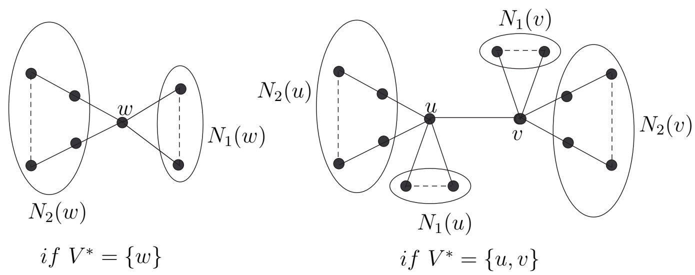

Figure 3.1 The structure of an extremal tree. $N_1(x)$ and $N_2(x)$ denote the set of pendent paths of length 1 and length 2 attached to x, respectively. $N_1(x)$ or $N_2(x)$ might be an empty set, $x \in \{u, v, w\}$.

Lemma 3.2 *For $\alpha > 0$, if $V^* = \{u, v\}$, let $d(u) = s \geq 3$ and $d(v) = t \geq 3$, then there exist pendent vertices in $N(u)$ and $N(v)$, respectively.*

Proof. By contradiction. Suppose there are no pendent vertices in $N(u)$ without loss of generality.

Case 1. For $0 < \alpha < 1$.

Let $T' = T^* - \bigcup_{x \in N(v)\backslash\{u\}} \{xv\} + \bigcup_{x \in N(v)\backslash\{u\}} \{xu\}$, then $T' \in \mathcal{T}_{n,m}$ and

$$
\begin{aligned}
&R_\alpha(T') - R_\alpha(T^*) \\
=&[(s+t-1)^\alpha - s^\alpha] \sum_{y \in N(u)\backslash\{v\}} d(y)^\alpha + [(s+t-1)^\alpha - t^\alpha] \sum_{x \in N(v)\backslash\{u\}} d(x)^\alpha \\
&+ (s+t-1)^\alpha - s^\alpha t^\alpha \\
\geq&[(s+t-1)^\alpha - t^\alpha](s-1) + [(s+t-1)^\alpha - s^\alpha](t-1) + (s+t-1)^\alpha - s^\alpha t^\alpha \\
\geq&(s+t-1)^{\alpha+1} - (s-1)s^\alpha - (t-1)t^\alpha - s^\alpha t^\alpha.
\end{aligned}
$$

Let $F_6(s,t) := (s+t-1)^{\alpha+1} - (s-1)s^\alpha - (t-1)t^\alpha - s^\alpha t^\alpha$, then

$$\frac{\partial^2 F_6(s,t)}{\partial s \partial t} = \alpha(\alpha+1)(s+t-1)^{\alpha-1} - \alpha^2 s^{\alpha-1}t^{\alpha-1} > \alpha^2[(s+t-1)^{\alpha-1} - s^{\alpha-1}t^{\alpha-1}] > 0,$$

since $s+t-1 \leq st$ for $s, t \geq 1$ and $\alpha \in (0,1)$. Thus $\frac{\partial F_6(s,t)}{\partial s} > \frac{\partial F_6(s,1)}{\partial s} = 0$, thereafter $F_6(s,t) > F_6(s,1) = 0$ for $s \geq 3$, a contradiction.

Case 2. For $\alpha \geq 1$.

Since $d(u) = s \geq 3$ and from Corollary 3.1, we have at least one pendent path of length 2 attached to u, namely uxy with $d(x) = 2,\ d(y) = 1$.

Let $T' = T - \{xy\} + \{vy\}$, then $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$, and

$$\begin{aligned} & R_\alpha(T') - R_\alpha(T^*) \\ =& [(t+1)^\alpha - t^\alpha] \sum_{w \in N(v)\setminus\{u\}} d(w)^\alpha + s^\alpha (t+1)^\alpha + (t+1)^\alpha \\ & + s^\alpha - 2^\alpha - (2s)^\alpha - (st)^\alpha \\ >& [(st+s)^\alpha - (st)^\alpha] - [(2s)^\alpha - s^\alpha] + (t+1)^\alpha - 2^\alpha \\ >& [(st+s)^\alpha - (st)^\alpha] - [(2s)^\alpha - s^\alpha] > 0, \end{aligned}$$

since the function $f(x) := (x+s)^\alpha - x^\alpha$ is monotonically increasing in $x \geq 3$ for $\alpha \geq 1$. We thus deduce a contradiction and complete the proof. ∎

Lemma 3.3 *For $\alpha \in (0, 1]$, we have $|V^*| = 1$.*
Proof. Suppose to the contrary that $V^* = \{u, v\}$. Assume $d(u) = t$, $d(v) = s$ and $t \geq s \geq 3$. By Lemma 3.2, there exists $z \in N(v)$ with $d(z) = 1$.

Let $T' = T^* - \sum_{y \in N(v)\setminus\{u,z\}} \{vy\} + \sum_{y \in N(v)\setminus\{u,z\}} \{uy\}$, then $T' \in \mathcal{T}_{n,m}(m \geq 2, n \geq 5)$, and

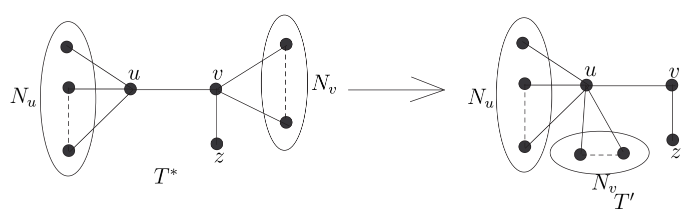

Figure 3.2 T^* and T' in Lemma 3.3, where N_u and N_v denote $N(u) \setminus \{v\}$ and $N(v) \setminus \{u, z\}$, respectively.

$$\begin{aligned} & R_\alpha(T') - R_\alpha(T^*) \\ =& [(t+s-2)^\alpha - t^\alpha] \sum_{x \in N(u)\setminus\{v\}} d(x)^\alpha + [(t+s-2)^\alpha - s^\alpha] \sum_{y \in N(v)\setminus\{u,z\}} d(y)^\alpha \\ & + (2t+2s-4)^\alpha - t^\alpha s^\alpha - s^\alpha + 2^\alpha \\ \geq& [(t+s-2)^\alpha - t^\alpha](t-1) + [(t+s-2)^\alpha - s^\alpha](s-2) \\ & + [(2t+2s-4)^\alpha - (ts)^\alpha] - (s^\alpha - 2^\alpha) \\ =& F_4(s, t, 1) > 0, \end{aligned}$$

by the last part of the proof of Lemma 2.5. We then deduce a contradiction and prove that $|V^*| = 1$ for $0 < \alpha \leq 1$. ∎

Theorem 3.4 *For $0 < \alpha \le 1$, let $T \in \mathcal{T}_{n,m}(m \ge 2, n \ge 5)$, then we have*

$$R_\alpha(T) \le 2^\alpha(m-1)[1+(n-m)^\alpha] + (n-2m+1)(n-2m).$$

Equality holds if and only if T has the structure of Figure 3.3.

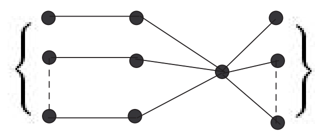

Figure 3.3 The structure of extremal trees for $0 < \alpha \le 1$.

Proof. If $n = 2m$ or $n \ge 2m+2$, then from Lemma 3.3, the structure of extremal tree T^* is unique and showed in Figure 3.3. And

$$R_\alpha(T^*) = 2^\alpha(m-1)[1+m^\alpha] + m^\alpha, \quad \text{if} \quad n = 2m;$$

$$R_\alpha(T^*) = 2^\alpha(m-1)[1+(n-m)^\alpha] + (n-2m+1)(n-2m), \quad \text{if} \quad n \ge 2m+2.$$

If $n = 2m+1$, then there are two possible structures of extremal trees showed in Figure 3.4. Since $R_\alpha(T_1) = 2^\alpha(m-1)[1+(m+1)^\alpha] + 2(m+1)^\alpha$, and $R_\alpha(T_2) = 2^\alpha m(1+m^\alpha)$, we have

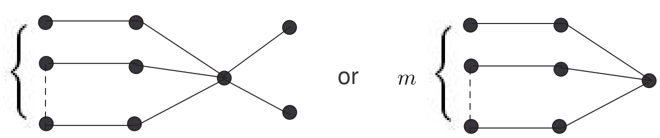

Figure 3.4 Possible structures of extremal trees with $n = 2m+1$ for $0 < \alpha \le 1$.

$R_\alpha(T_1) - R_\alpha(T_2) = 2^\alpha[m(m+1)^\alpha - m^{\alpha+1} - 1] + (2-2^\alpha)(m+1)^\alpha$. Define $g(x) := x(x+1)^\alpha - x^{\alpha+1} - 1$, then for $0 < \alpha \le 1$,

$$\begin{aligned} g'(x) =& (\alpha+1)[(x+1)^\alpha - x^\alpha] - \alpha(x+1)^{\alpha-1} \\ >& \alpha(\alpha+1)(x+1)^{\alpha-1} - \alpha(x+1)^{\alpha-1} = \alpha(x+1)^{\alpha-1} > 0, \end{aligned}$$

which means $g(x)$ is monotonically increasing in $x \ge 1$ for $0 < \alpha \le 1$, thereby $g(m) \ge g(2) > f(1) = 0$. Thus $R_\alpha(T_1) - R_\alpha(T_2) > 0$, which completes the proof.

Remark: For $T \in \mathcal{T}_{n,m}(m \ge 2, n \ge 5)$ we have obtained the maximum value of the general Randić index and shown the extremal tree for $0 < \alpha \le 1$. And for $\alpha > 1$, we have the structure in Corollary 3.1. But for the case $\alpha < 0$, it is rather complicated, and will be studied further.

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