On the tree with maximum general Randić Index

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Abstract. The general Randić index $R_{-\alpha}(G)$ of a graph G, defined by a real number α, is 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. In this paper, we have discussed some properties of the Max Tree which has the maximum general Randić index $R_{-\alpha}$, here $\alpha \in (\alpha_0, 2)$, and α_0 is some real number in the interval $(1.2961, 1.2962)$. Based on these properties, we are able to obtain the structure of the Max Tree among all trees of order $k \geq 3$. Thus the maximal value of $R_{-\alpha}$ follows easily.

Keywords: general Randić index; Max Tree; big degree vertex.

1 Introduction

Let k represent the order of a tree T all through this paper. A *suspended path* of length t rooted at z is a path $xy_1y_2\cdots y_{t-1}z$ with $d(x) = 1$, $d(y_j) = 2$(for all $1 \leq j \leq t-1$), $d(z) \geq 3$. A *Single Center Tree* consists of one vertex ω with n distinguish suspended paths of length 2 rooted at ω, where $n \geq 3$, we call it SCT for short; if there is $n-1$ distinguish suspended paths of length 2 and one suspended path of length 3 rooted at vertex ω, then they form an *Abnormal Single Center Tree*, which is called $ASCT$ for short. A *Double Center Tree* consists of two adjacent vertices ω and ω_1, with $n-1$ distinguish suspended paths of length 2 rooted at ω and $m-1$ distinguish suspended paths of length 2 rooted at ω_1, where $n \geq m \geq 3$, we call it DCT for short; if there is $n-1$ distinguish suspended paths of length 2 rooted at ω and $m-2$ distinguish suspended paths of length 2, one suspended path of length 3 rooted at ω_1, then they form an *Abnormal*

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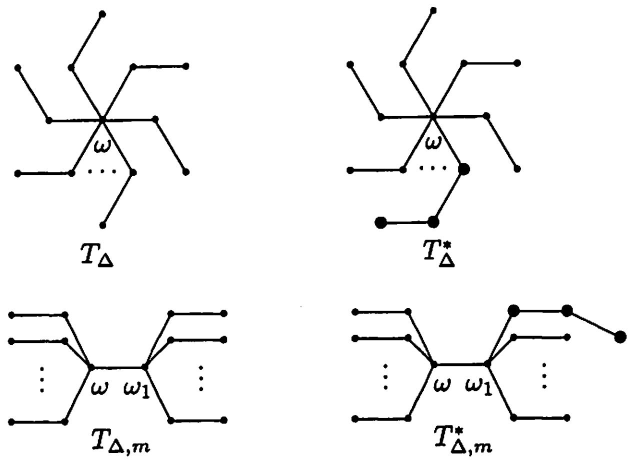
Double Center Tree, which is called *ADCT* for short. Clearly, ω is always the vertex with maximum degree, so $d(\omega) = n = \Delta$, where Δ denotes the maximum degree. In the following, we use T_Δ, T^*_Δ, $T_{\Delta,m}$ and $T^*_{\Delta,m}$ to denote SCT, ASCT, DCT and ADCT separately. These four trees are shown in the following picture:



In 1975 Randić[7] proposed a pair of topological indices $R_{-\frac{1}{2}}(G)$ and $R_{-1}(G)$ in order to measure molecular branching. Thereafter, Paul Erdös generalized[2] the index by changing $\frac{1}{2}$ to an arbitrary real number α, which stimulated many other colleagues to study the general Randić index $R_{-\alpha}((G)) = \sum_{uv\in E(G)} (d(u)d(v))^{-\alpha}$.

People want to get the extremal value of general Randić index and the extremal trees. The minimal value and the Min Tree have been already solved completely[4]. Until now, there are many papers about the Max Tree, and most of the problems have been solved[5]. The result is:

α	the Max Tree T
$(-\infty, -2]^*$	balance double star for $k \geq 8$
$(-2, -1)$	star or double star
$[-1, 0)$	star
$(0, \frac{1}{2}]$	path
$(\frac{1}{2}, 2)$	
$[2, +\infty)$	path for $k \leq 6$; $T_{\frac{k-1}{2}}$ or $T^*_{\frac{k}{2}-1}$ for $k \geq 7$

$*$ means for $k \leq 7$, the Max Tree depends on α.

Only the interval $(\frac{1}{2}, 2)$ is still undetermined. Work [6] is about the maximal value of R_{-1}. Recently, Balister, Bollobás and Gerke have given an upper bound of the general Randić index for $\forall\alpha > 0$. In their paper[1], they gave the minimal constant $\beta_0(\alpha)$ which satisfies $R_{-\alpha} \leq \beta_0(k+1)$, and this bound is sharp up to an additive constant since they have found infinitely many trees with $R_{-\alpha} \geq \beta_0(k-1)$. This kind of trees are called the *optimal trees*, and the index values of them are maximal or close to the maximal value, however they did not make a sure answer. Besides the structure of the optimal tree only exists for special k.

In this paper we will partially fill up the gap in the above tabular. In section 2, we obtain some important properties of the Max Tree. In section 3, we discuss two cases based on the properties and get the structure of tree with maximum $R_{-\alpha}$ in each condition. In section 4, we compare the results in the two cases in section 3 and for every order $k \geq 3$ finally obtain the maximal value of the general Randić index $R_{-\alpha}$ when $\alpha \in (\alpha_0, 2)$, where α_0 is some real number in the interval $(1.2961, 1.2962)$.

2 Properties for the Max Tree

Firstly, it is clear that paths have maximum $R_{-\alpha}$ for $k \leq 6$ when $\alpha > 1$, and the maximal value is $\frac{k-3}{4^\alpha} + \frac{1}{2^{\alpha-1}}$, thus we assume $k \geq 7$ all through the next of the paper. It is necessary to describe an important property for the Max Tree when $\alpha > 1$.

Lemma 2.1. [3] *If T is the Max Tree for the general Randić index $R_{-\alpha}$ when $\alpha > 1$, then*

(1) *any leaf is connected with the vertex of degree* 2.

(2) *every vertex of degree* 2 *must appear on a suspended path.*

(3) *all the suspended paths are of length* 2, *except for at most one with length* 3.

By the above lemma, one could easily see that in the Max Tree the maximum degree $\Delta \geq 3$. We call a vertex the *big degree vertex* if it is of degree at least 3. $BD(z)$ means the number of big degree vertices adjacent to vertex z. Then we describe the next property:

Lemma 2.2. *There exists a real number $\alpha_0 \in (1.2961, 1.2962)$, s.t., for any $\alpha > \alpha_0$, if T is the Max Tree for the general Randić index $R_{-\alpha}$ and $\omega \in V(T)$ with $d(\omega) = \Delta$, then $BD(\omega) \leq 1$.*

Proof. By contradiction. Assume $BD(\omega) \geq 2$, that is ω has at least two big degree vertices adjacent to it. Among all these big degree vertices, two are denoted by ω_1 and ω_2. Here without loss of generality, we suppose $d(\omega_1) = m \geq d(\omega_2) = n \geq 3$. Besides, let y_t $(1 \leq t \leq \Delta - 2)$ denote the vertices adjacent to ω other than ω_1 and ω_2, x_{1i} be the vertices adjacent to ω_1 other than ω and x_{2j} be the vertices adjacent to ω_2 other than ω, where $1 \le i \le m-1$, $1 \le j \le n-1$.

Delete ω_1, ω_2, let all x_{1i}, x_{2j} be joined to ω and add one suspended path of length 2 to ω, so we get a new tree T' of the same order. By lemma2.1 we have $d(y_t)$, $d(x_{1i})$, $d(x_{2j}) \ge 2$, thus the difference:

$$\begin{aligned}
& R_{-\alpha}(T) - R_{-\alpha}(T') \\
= & \left(\frac{1}{\Delta^\alpha} - \frac{1}{(\Delta+m+n-3)^\alpha}\right) \sum_{t=1}^{\Delta-2} \frac{1}{d(y_t)^\alpha} \\
& + \left(\frac{1}{m^\alpha} - \frac{1}{(\Delta+m+n-3)^\alpha}\right) \sum_{i=1}^{m-1} \frac{1}{d(x_{1i})^\alpha} \\
& + \left(\frac{1}{n^\alpha} - \frac{1}{(\Delta+m+n-3)^\alpha}\right) \sum_{j=1}^{n-1} \frac{1}{d(x_{2j})^\alpha} \\
& + \frac{1}{\Delta^\alpha}\left(\frac{1}{m^\alpha} + \frac{1}{n^\alpha}\right) - \frac{1}{(2(\Delta+m+n-3))^\alpha} - \frac{1}{2^\alpha} \\
\le & \left(\frac{1}{\Delta^\alpha} - \frac{1}{(\Delta+m+n-3)^\alpha}\right) \frac{\Delta-2}{2^\alpha} \\
& + \left(\frac{1}{m^\alpha} - \frac{1}{(\Delta+m+n-3)^\alpha}\right) \frac{m-1}{2^\alpha} \\
& + \left(\frac{1}{n^\alpha} - \frac{1}{(\Delta+m+n-3)^\alpha}\right) \frac{n-1}{2^\alpha} \\
& + \frac{1}{\Delta^\alpha}\left(\frac{1}{m^\alpha} + \frac{1}{n^\alpha}\right) - \frac{1}{(2(\Delta+m+n-3))^\alpha} - \frac{1}{2^\alpha} \\
= & \frac{1}{2^\alpha}\left[\frac{\Delta-2}{\Delta^\alpha} + \frac{m-1}{m^\alpha} + \frac{n-1}{n^\alpha} + \left(\frac{2}{\Delta}\right)^\alpha \left(\frac{1}{m^\alpha} + \frac{1}{n^\alpha}\right)\right. \\
& \left. - \frac{1}{(\Delta+m+n-3)^{\alpha-1}} - 1\right] \\
= & f(\Delta, m, n; \alpha)
\end{aligned}$$

We need to find α which keeps the inequality $f(\Delta, m, n; \alpha) < 0$.

Let set $A = \{\alpha \mid f(\Delta, m, n; \alpha) = 0, \Delta \ge m \ge n \ge 3, \Delta, m, n \in \mathbb{N}\}$. Define $\alpha_0^* = \sup_{\alpha \in A} \alpha$. We show the existence of α_0^* in two steps.

(I) To show $f(\Delta, m, n; 1.2962) < 0$.

Since

$$\begin{aligned}\frac{\partial f}{\partial m} &= \frac{1.2962\left(1-\left(\frac{2}{\Delta}\right)^{1.2962}\right)-0.2962m}{2^{1.2962}\times m^{2.2962}}+\frac{0.2962}{(2(\Delta+m+n-3))^{1.2962}}\\ &\le \frac{1.2962\left(1-\left(\frac{2}{\Delta}\right)^{1.2962}\right)-0.2962m}{2^{1.2962}\times m^{2.2962}}+\frac{0.2962}{(2(\Delta+m))^{1.2962}}\\ &= Z(\Delta,m)\end{aligned}$$

Notice that

$$\begin{aligned}\frac{\partial Z(\Delta,m)}{\partial\Delta} &= \frac{1.2962}{2^{1.2962}\times\Delta^{2.2962}}\left(\frac{1.2962\times 2^{1.2962}}{m^{2.2962}}-\frac{0.2962}{(1+\frac{m}{\Delta})^{2.2962}}\right)\\ &\le \frac{1.2962}{2^{1.2962}\times\Delta^{2.2962}}\left(\frac{1.2962\times 2^{1.2962}}{m^{2.2962}}-\frac{0.2962}{2^{2.2962}}\right)<0\end{aligned}$$

provides $m\ge 6$. Thus when $m\ge 6$, we have

$$Z(\Delta,m)\le Z(m,m)=\frac{1}{(2m)^{1.2962}}z(m)$$

Here $z(m)=\frac{1.2962\left(1-\left(\frac{2}{m}\right)^{1.2962}\right)}{m}-0.2962\left(1-\frac{1}{2^{1.2962}}\right)$. Then easily we get $\frac{dz(m)}{dm}<0$ when $m\ge 4$. But $z(6)<0$, so when $m\ge 6$, $z(m)\le z(6)<0$, then we have $\frac{\partial f}{\partial m}\le Z(\Delta,m)\le Z(m,m)=\frac{1}{(2m)^{1.2962}}z(m)<0$, when $m\ge 6$.

Thus $f(\Delta,m,n;1.2962)$ is monotone decreasing in m when $m\ge 6$. Noticing the symmetry of m and n in function $f(\Delta,m,n;1.2962)$, the same conclusion holds for n. Then we discuss in several cases:

case 1. $\Delta\ge m\ge n\ge 6$

Clearly $f(\Delta,m,n;1.2962)\le f(\Delta,6,6;1.2962)$. By **Lagrange Mean Value Theorem**, we have

$$\begin{aligned}&\frac{df(\Delta,6,6;1.2962)}{d\Delta}\\ =\ &\frac{1}{2^{1.2962}}\left(\frac{2\times 1.2962\left(1-\left(\frac{1}{3}\right)^{1.2962}\right)}{\Delta^{2.2962}}+\left(\frac{0.2962}{(\Delta+9)^{1.2962}}-\frac{0.2962}{\Delta^{1.2962}}\right)\right)\\ =\ &\frac{1}{2^{1.2962}}\left(\frac{2\times 1.2962\left(1-\left(\frac{1}{3}\right)^{1.2962}\right)}{\Delta^{2.2962}}-\frac{9\times 1.2962\times 0.2962}{\xi^{2.2962}}\right)\\ <\ &\frac{1.2962}{2^{1.2962}}\left(\frac{2\left(1-\left(\frac{1}{3}\right)^{1.2962}\right)}{\Delta^{2.2962}}-\frac{9\times 0.2962}{(\Delta+9)^{2.2962}}\right)\end{aligned}$$

where $\xi \in (\Delta, \Delta+9)$.

Then it would be easy to get that when $\Delta \geq 33$, $\frac{df(\Delta,6,6;1.2962)}{d\Delta} < 0$. Hence $f(\Delta,6,6;1.2962) \leq f(33,6,6;1.2962) < 0$ when $\Delta \geq 33$. For the rest case $6 \leq \Delta \leq 32$, substitute these values for Δ in $f(\Delta,6,6;1.2962)$ directly, and we would also obtain $f(\Delta,6,6;1.2962) < 0$.

case 2. $\Delta \geq m \geq 6,\ 3 \leq n \leq 5$

We have previously shown that $f(\Delta,m,n;1.2962) \leq f(\Delta,6,n,1.2962)$. Notice that function $\frac{x-1}{x^{1.2962}}$ ($x \in \mathbb{Z}^+$, here $\mathbb{Z}^+$ represents the positive integer set) is monotone increasing when $x \leq 4$ and is monotone decreasing when $x \geq 4$. Maximizing each part of $f(\Delta,6,n,1.2962)$ by substituting different values for n, we can obtain that

$$\begin{aligned} f(\Delta,6,n,1.2962) &< \frac{1}{2^{1.2962}}\left[\frac{\Delta-2}{\Delta^{1.2962}}+\frac{5}{6^{1.2962}}+\frac{3}{4^{1.2962}}+\left(\frac{2}{\Delta}\right)^{1.2962}\times\right.\\ &\quad \left.\left(\frac{1}{6^{1.2962}}+\frac{1}{3^{1.2962}}\right)-\frac{1}{(\Delta+8)^{0.2962}}-1\right]\\ &= F(\Delta) \end{aligned}$$

By **Lagrange Mean Value Theorem**, we have

$$\begin{aligned} \frac{dF(\Delta)}{d\Delta} &= \frac{1.2962}{2^{1.2962}}\left(\frac{2-\left(\frac{1}{3}\right)^{1.2962}-\left(\frac{2}{3}\right)^{1.2962}}{\Delta^{2.2962}}-\frac{8\times 0.2962}{\xi^{2.2962}}\right)\\ &< \frac{1.2962}{2^{1.2962}}\left(\frac{2-\left(\frac{1}{3}\right)^{1.2962}-\left(\frac{2}{3}\right)^{1.2962}}{\Delta^{2.2962}}-\frac{8\times 0.2962}{(\Delta+8)^{2.2962}}\right)<0 \end{aligned}$$

provides $\Delta \geq 23$, where $\xi \in (\Delta, \Delta+8)$. But notice $F(25) < 0$, we have $f(\Delta,6,n,1.2962) < F(\Delta) < 0$ when $\Delta \geq 25$.

For $3 \leq \Delta \leq 24$, substitute values of $3 \leq \Delta \leq 24,\ 3 \leq n \leq 5$ for Δ, n in function $f(\Delta,6,n,1.2962)$, it is not hard to get $f(\Delta,6,n,1.2962) < 0$.

case 3. $3 \leq n \leq m \leq 5, \Delta \geq 6$

Maximize each part in $f(\Delta,m,n;1.2962)$ by substituting different values for m, n, then

$$\begin{aligned} f(\Delta,m,n;1.2962) &< \frac{1}{2^{1.2962}}\left[\frac{\Delta-2}{\Delta^{1.2962}}+\frac{4-1}{4^{1.2962}}+\frac{4-1}{4^{1.2962}}+\left(\frac{2}{\Delta}\right)^{1.2962}\times\right.\\ &\quad \left.\frac{2}{3^{1.2962}}-\frac{1}{(\Delta+5+5-3)^{0.2962}}-1\right]\\ &= F(\Delta) \end{aligned}$$

By **Lagrange Mean Value Theorem**, we have

$$\begin{aligned}\frac{dF(\Delta)}{d\Delta} &= \frac{1.2962}{2^{1.2962}}\left(\frac{2\left(1-\left(\frac{2}{3}\right)^{1.2962}\right)}{\Delta^{2.2962}} - \frac{7\times 0.2962}{\xi^{2.2962}}\right)\\ &\leq \frac{1.2962}{2^{1.2962}}\left(\frac{2\left(1-\left(\frac{2}{3}\right)^{1.2962}\right)}{\Delta^{2.2962}} - \frac{7\times 0.2962}{(\Delta+7)^{2.2962}}\right) < 0\end{aligned}$$

provides $\Delta \geq 15$, where $\xi \in (\Delta, \Delta+7)$. But notice $F(64) < 0$, we have $f(\Delta, m, n; 1.2962) < F(\Delta) < 0$ when $\Delta \geq 64$.

For the undiscussed case $6 \leq \Delta \leq 63$, $3 \leq n \leq m \leq 5$, one might calculate the values of $f(\Delta, m, n; 1.2962)$ one by one, and $f(\Delta, m, n; 1.2962) < 0$ holds, too.

case 4. $3 \leq n \leq m \leq \Delta \leq 5$

Substitute values for Δ, m, n, the readers could easily see $f(\Delta, m, n; 1.2962) < 0$ holds.

Therefore $f(\Delta, m, n; 1.2962) < 0$.

(II) To explain $f(\Delta, m, n; \alpha)$ is monotone decreasing in α when $\alpha > 1$.

It is equivalent to show $h(\Delta, m, n; \alpha)$ is monotone decreasing in α when $\alpha > 1$, here $h(\Delta, m, n; \alpha) = 2^\alpha f(\Delta, m, n; \alpha)$.

Let $s = \Delta + m + n - 3$, easily one may see

$$\begin{aligned}\frac{\partial h}{\partial \alpha} &= \left(\frac{2}{\Delta}\right)^\alpha \left[\left(\frac{1}{m^\alpha}+\frac{1}{n^\alpha}\right)\ln\left(\frac{2}{\Delta}\right) - \left(\frac{\ln m}{m^\alpha}+\frac{\ln n}{n^\alpha}\right)\right] + \\ &\quad \frac{\ln s}{s^{\alpha-1}} - (\Delta-2)\frac{\ln\Delta}{\Delta^\alpha} - (m-1)\frac{\ln m}{m^\alpha} - (n-1)\frac{\ln n}{n^\alpha}\end{aligned}$$

Notice $\Delta \geq m \geq n \geq 3$, the former term is less than 0. So we only need to analyze

$$\frac{\ln s}{s^{\alpha-1}} - (\Delta-2)\frac{\ln\Delta}{\Delta^\alpha} - (m-1)\frac{\ln m}{m^\alpha} - (n-1)\frac{\ln n}{n^\alpha} \qquad (*)$$

Clearly $\Delta \leq s-3$. It can be shown that function $\frac{\ln x}{x^\alpha}$ is monotone decreasing in x when $x \geq 3$, thus

$$\begin{aligned}(*) &\leq \frac{\ln s}{s^{\alpha-1}} - (\Delta-2)\frac{\ln\Delta}{\Delta^\alpha} - (m-1)\frac{\ln\Delta}{\Delta^\alpha} - (n-1)\frac{\ln\Delta}{\Delta^\alpha}\\ &= \frac{\ln\Delta}{\Delta^\alpha}\left(\frac{s\ln s}{\ln\Delta}\times\left(\frac{\Delta}{s}\right)^\alpha - (s-1)\right)\\ &< \frac{\ln\Delta}{\Delta^\alpha}\left(\frac{s\ln s}{\ln\Delta}\times\frac{\Delta}{s} - (s-1)\right)\end{aligned}$$

$$\begin{aligned} &\le \frac{\ln\Delta}{\Delta^\alpha}\left(\ln s \times \frac{s-3}{\ln(s-3)} - (s-1)\right) \\ &= \frac{\ln\Delta}{\Delta^\alpha \ln(s-3)}\left((s-3)\ln s - (s-1)\ln(s-3)\right) \end{aligned}$$

Let $G(s) = (s-3)\ln s - (s-1)\ln(s-3)$, since $\frac{d^2G(s)}{ds^2} > 0$, we know $G(s)$ is convex. Then notice $G(6) < 0$ and $\lim_{s\to+\infty} G(s) = -\infty$, we conclude that $G(s) \le 0$.

Therefore, $\frac{\partial h(\Delta,m,n;\alpha)}{\partial\alpha} < 0$ which implies $h(\Delta,m,n;\alpha)$ is monotone decreasing in α when $\alpha > 1$, and so does $f(\Delta,m,n;\alpha)$.

Observing monotonicity of $f(\Delta,m,n;\alpha)$ in α and $f(\Delta,m,n;1.2962) < 0$, one could deduce that $\forall\alpha \ge 1.2962$, $f(\Delta,m,n;\alpha) \le f(\Delta,m,n;1.2962) < 0$. So $\forall\alpha \in A$, $\alpha < 1.2962$, then 1.2962 is an upper bound for all $\alpha \in A$; besides notice $f(16,5,5;1.2961) > 0$, by continuity of f, we know that A is nonempty and $\alpha_0^* = \sup_{\alpha\in A}\alpha$ does exist. Clearly $\alpha_0^* \in (1.2961, 1.2962)$.

Notice $R_{-\alpha}(T) - R_{-\alpha}(T') \le f(\Delta,m,n;\alpha)$ with the equality holds if and only if $d(y_t) = d(x_{1i}) = d(x_{2j})(t = 1,2,\cdots,\Delta-2; i = 1,2,\cdots,m-1; j = 1,2\cdots,n-1)$. So when the equality holds and $\Delta = 16, m = n = 5$, $R_{-1.2961}(T) - R_{-1.2961}(T') = f(16,5,5;1.2961) > 0$, therefore take $\alpha_0 = \alpha_0^*$, then the lemma is clearly true. □

In the following paper, symbol ω always denotes one of the maximum degree vertex in the Max Tree T and we assume that α_0, which belongs to the interval $(1.2961, 1.2962)$, always represents the real number obtained in the above lemma.

3 The Max Tree structure

In order to obtain the structure of the Max Tree for $R_{-\alpha}$, where $\alpha \in (\alpha_0, 2)$, it follows from lemma2.2 that the discussion should be separated into two cases. And in each case to find the tree with the maximal index value.

Case1. $BD(\omega) = 0$

This case might be easily dealt by lemma2.1. Notice we have

$$\begin{aligned} R_{-\alpha}(T_\Delta) &= \frac{\Delta}{(2\Delta)^\alpha} + \frac{\Delta}{2^\alpha} \\ R_{-\alpha}(T_\Delta^*) &= \frac{\Delta}{(2\Delta)^\alpha} + \frac{\Delta}{2^\alpha} + \frac{1}{4^\alpha} \end{aligned}$$

thus

Theorem 3.1. *Let ω denote the vertex with maximum degree and $T^0 = \{T \mid |V(T)| = k, BD(\omega) = 0\}$, then the maximum general Randić index $R_{-\alpha}$ where $\alpha \in (\alpha_0, 2)$ among trees in T^0 is :*

when k is odd: $R_{-\alpha}\left(T_{\frac{k-1}{2}}\right)$;
when k is even: $R_{-\alpha}\left(T^*_{\frac{k}{2}-1}\right)$.

We omit the proof because it is quite easy.

Case2. $BD(\omega) = 1$

Let ω_1 denote the unique big degree vertex in T which is adjacent to ω, and $d(\omega_1) = m \geq 3$. Clearly the order k of T is at least 10.

When k is even, T is just a DCT, thus there is a clear equation $\Delta + m = \frac{k}{2} + 1$; but when k is odd, by lemma2.1 there exist exactly one suspended path of length 3. Clearly, we might assume the tree is a ADCT without loss of generality.

Consider the difference:

$$\begin{aligned}
& R_{-\alpha}(T_{\Delta,m}) - R_{-\alpha}(T_{\Delta+1,m-1}) \\
= \ & \left(\frac{\Delta-1}{(2\Delta)^\alpha} - \frac{\Delta}{(2(\Delta+1))^\alpha}\right) - \left(\frac{m-2}{(2(m-1))^\alpha} - \frac{m-1}{(2m)^\alpha}\right) + \\
& \left(\frac{1}{(\Delta m)^\alpha} - \frac{1}{((\Delta+1)(m-1))^\alpha}\right) \\
= \ & g(\Delta, m; \alpha)
\end{aligned}$$

Then we have the following lemma:

Lemma 3.2. *When* $\alpha \in (\alpha_0, 2)$, $g(\Delta, m; \alpha) < 0$ *holds if* Δ, m *satisfy the following conditions:*

$$\begin{cases} \Delta \geq m \geq 8 \\ \Delta \geq 8, \ m = 7 \\ \Delta \geq 11, \ m = 6 \\ \Delta \geq 68, \ m = 5 \end{cases}$$

Proof. For any $\alpha \in (\alpha_0, 2)$, consider

$$G(\Delta, m; \alpha) = g(\Delta, m; \alpha) + \left(\frac{1}{((\Delta+1)(m-1))^\alpha} - \frac{1}{(\Delta m)^\alpha}\right)$$

Notice that $\frac{1}{((\Delta+1)(m-1))^\alpha} > \frac{1}{(\Delta m)^\alpha}$, thus it will follow $g(\Delta, m; \alpha) < 0$ as long as $G(\Delta, m; \alpha) \leq 0$. Let $F(x; \alpha) = \frac{x}{(2(x+1))^\alpha}$, then

$$G(\Delta, m; \alpha) = F(\Delta - 1; \alpha) - F(\Delta; \alpha) - F(m-2; \alpha) + F(m-1; \alpha)$$

Discuss in cases described in the lemma.

(1) $\Delta \geq m \geq 8$
We know $\frac{\partial F(x;\alpha)}{\partial x} = F'(x; \alpha)$ is monotone increasing in x when $x \geq 7$.

If $m-2 \geq 7$, by **Lagrange Mean Value Theorem**, it follows that:

$F(\Delta;\alpha)-F(\Delta-1;\alpha) = F'(\xi_1;\alpha) > F'(\xi_2;\alpha) = F(m-1;\alpha)-F(m-2;\alpha)$

where $\xi_1 \in (\Delta-1,\Delta)$ and $\xi_2 \in (m-2,m-1)$, thus $G(\Delta,m;\alpha) < 0$.
If $m = 8$, notice $\Delta \geq 8$, which implies

$$F(\Delta-1;\alpha) - F(\Delta;\alpha) \leq F(7;\alpha) - F(8;\alpha)$$

consequently

$$\begin{aligned} G(\Delta,8;\alpha) &\leq F(7;\alpha) - F(8;\alpha) - F(6;\alpha) + F(7;\alpha) \\ &= \frac{14}{16^\alpha} - \frac{8}{18^\alpha} - \frac{6}{14^\alpha} = S_1(\alpha) \end{aligned}$$

We need to show $S_1(\alpha) < 0$.
By mathematica software, we could draw the picture of $S_1(\alpha)$ in interval $(1,2)$, as shown in Figure 1.

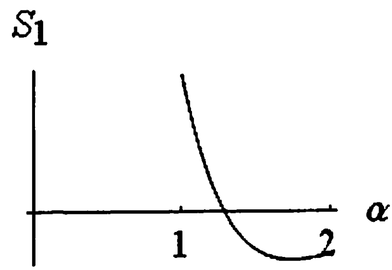


Figure 1: The image of $S_1(\alpha)$

One might easily see there is only one root of $S_1(\alpha) = 0$, then notice that $S_1(1.2961) < 0$ and $S_1(2) < 0$, we conclude that $S_1(\alpha) < 0$ when $\alpha \in (\alpha_0, 2) \subset (1.2961, 2)$. Hence $G(\Delta, 8;\alpha) < 0$ for $\Delta \geq 8$.

(2) $\Delta \geq 8,\ m = 7$

$$G(\Delta,7;\alpha) \leq \frac{9}{20^\alpha} - \frac{10}{22^\alpha} - \frac{5}{12^\alpha} + \frac{6}{14^\alpha} = S_2(\alpha)$$

when $\Delta \geq 10$.
As the proof of $S_1(\alpha) < 0$, we firstly obtain the picture of $S_2(\alpha)$ in interval $(1,2)$ by mathematica software, which is similar as the

picture shown in Figure 1. Then notice that $S_2(1.2961) < 0$ and $S_2(2) < 0$, we conclude that $S_2(\alpha) < 0$ for $\alpha \in (\alpha_0, 2) \subset (1.2961, 2)$. Hence $G(\Delta, 7; \alpha) < 0$ for $\Delta \geq 10$. For $\Delta = 8, 9$, we could directly prove $g(\Delta, 7; \alpha) < 0$ holds by the same method, the proof is omitted.

(3) $\Delta \geq 11, m = 6$

$$G(\Delta, 6; \alpha) \leq \frac{13}{28^\alpha} - \frac{14}{30^\alpha} - \frac{4}{10^\alpha} + \frac{5}{12^\alpha} = S_3(\alpha)$$

when $\Delta \geq 14$.

As the proof of $S_1(\alpha) < 0$, we firstly obtain the picture of $S_3(\alpha)$ in interval $(1, 2)$ by mathematica software, which is similar as the picture shown in Figure 1. Then notice that $S_3(1.2961) < 0$ and $S_3(2) < 0$, we conclude that $S_3(\alpha) < 0$ for $\alpha \in (\alpha_0, 2) \subset (1.2961, 2)$. Hence $G(\Delta, 6; \alpha) < 0$ for $\Delta \geq 14$. One could verify that $g(\Delta, 6; \alpha) < 0$ also holds when $\Delta = 11, 12, 13$ by the same method.

(4) $\Delta \geq 68, m = 5$

$$G(\Delta, 5; \alpha) \leq \frac{95}{192^\alpha} - \frac{96}{194^\alpha} - \frac{3}{8^\alpha} + \frac{4}{10^\alpha} = S_4(\alpha)$$

when $\Delta \geq 96$.

As the proof of $S_1(\alpha) < 0$, we firstly obtain the picture of $S_4(\alpha)$ in interval $(1, 2)$ by mathematica software, which is similar as the picture shown in Figure 1. Then notice that $S_4(1.2961) < 0$ and $S_4(2) < 0$, we conclude that $S_4(\alpha) < 0$ for $\alpha \in (\alpha_0, 2) \subset (1.2961, 2)$. Hence $G(\Delta, 5; \alpha) < 0$ for $\Delta \geq 96$. For $68 \leq \Delta \leq 95$, by the same method we can get $g(\Delta, 5; \alpha) < 0$, too.

However, one should observe that it is impossible to determine the signs of $g(7, 7; \alpha)$, $g(\Delta, 6; \alpha)$ for $6 \leq \Delta \leq 10$, $g(\Delta, 5; \alpha)$ for $5 \leq \Delta \leq 67$, $g(\Delta, 4; \alpha)$ and $g(\Delta, 3; \alpha)$. □

Now we can give the structure of the tree with maximum general Randicć index in this case. Notice we have

$$\begin{aligned} R_{-\alpha}(T_{\Delta,m}) &= \frac{\Delta - 1}{(2\Delta)^\alpha} + \frac{m-1}{(2m)^\alpha} + \frac{1}{(\Delta m)^\alpha} + \frac{\Delta + m - 2}{2^\alpha} \\ R_{-\alpha}(T^*_{\Delta,m}) &= \frac{\Delta - 1}{(2\Delta)^\alpha} + \frac{m-1}{(2m)^\alpha} + \frac{1}{(\Delta m)^\alpha} + \frac{\Delta + m - 2}{2^\alpha} + \frac{1}{4^\alpha} \end{aligned}$$

thus

Theorem 3.3. *Let ω be the vertex with maximum degree and set $T^1 = \{T \mid |V(T)| = k, BD(\omega) = 1\}$, then the maximum general Randić index*

$R_{-\alpha}$ *where* $\alpha \in (\alpha_0, 2)$ *among trees in* $\mathcal{T}^1$ *is :*
when k *is even:*

$$\begin{cases} \max\limits_{3\le m\le 6}\left\{R_{-\alpha}\left(T_{\frac{k}{2}+1-m,m}\right)\right\} & 10\le k\le 30, k\ne 26 \\ \max\limits_{3\le m\le 7}\left\{R_{-\alpha}\left(T_{14-m,m}\right)\right\} & k=26 \\ \max\limits_{3\le m\le 5}\left\{R_{-\alpha}\left(T_{\frac{k}{2}+1-m,m}\right)\right\} & 32\le k\le 142 \\ \max\limits_{3\le m\le 4}\left\{R_{-\alpha}\left(T_{\frac{k}{2}+1-m,m}\right)\right\} & k\ge 144 \end{cases}$$

when k *is odd:*

$$\begin{cases} \max\limits_{3\le m\le 6}\left\{R_{-\alpha}\left(T^*_{\frac{k+1}{2}-m,m}\right)\right\} & 11\le k\le 31, k\ne 27 \\ \max\limits_{3\le m\le 7}\left\{R_{-\alpha}\left(T^*_{14-m,m}\right)\right\} & k=27 \\ \max\limits_{3\le m\le 5}\left\{R_{-\alpha}\left(T^*_{\frac{k+1}{2}-m,m}\right)\right\} & 33\le k\le 143 \\ \max\limits_{3\le m\le 4}\left\{R_{-\alpha}\left(T^*_{\frac{k+1}{2}-m,m}\right)\right\} & k\ge 145 \end{cases}$$

Proof. We firstly assume k is even, then $\Delta + m = \frac{k}{2} + 1$.

Clearly, by lemma2.1 the structure of the Max Tree should be DCT. But by lemma3.2, we know $g(\Delta, m; \alpha) < 0$ when $\Delta \ge m \ge 8$, thus the tree with maximum general Randić index in $\mathcal{T}^1$ must be among $T_{\Delta,m}$ where $3 \le m \le 7$. Distinguish in several cases.

(1) $10 \le k \le 30$, $k \ne 26$
Since $6 \le \Delta+m \le 16$, $\Delta+m \ne 14$, when $m = 7$, we have $8 \le \Delta \le 9$. By lemma3.2, we can see that $T_{\Delta,7}$ could not be the Max Tree. When $m = 6$, $6 \le \Delta \le 10$, $m \ne 8$, because the sign of $g(\Delta, 6; \alpha)$ when $\Delta \le 10$ is undetermined, we could not ascertain whether $T_{\Delta,6}$ is the Max Tree. Similarly, $T_{\Delta,m} (3 \le m \le 5)$ could not be excluded too.

(2) $k = 26$
Comparing with the above case, there is only a difference, that is $T_{\Delta,7}$ is included since the sign of $g(7, 7; \alpha)$ is uncertain.

(3) $32 \le k \le 142$
Notice $17 \le \Delta + m \le 72$, then $T_{\Delta,6}$ should be clearly excluded, since when $m = 6$, we have $\Delta \ge 11$.

(4) $k \ge 144$
Clearly $\Delta + m \ge 73$, so when $m = 5$, we have $\Delta \ge 68$ which implies $g(\Delta, 5; \alpha) < 0$. Therefore $T_{\Delta,5}$ could not be the Max Tree.

The result for odd k follows clearly. □

4 The Maximal value of the general Randić index $R_{-\alpha}$

By **Theorem3.1** and **Theorem3.3**, we may get the main theorem in this paper:

Theorem 4.1. *For $\alpha \in (\alpha_0, 2)$, the maximum value of the general Randić index $R_{-\alpha}$ of trees with order $k \geq 7$ is:*
when k is odd: $R_{-\alpha}\left(T_{\frac{k-1}{2}}\right)$;
when k is even:

$$\begin{cases} R_{-\alpha}\left(T_3^*\right) & k = 8 \\ \max\left\{\max\limits_{3\leq m\leq 6}\left\{R_{-\alpha}\left(\frac{k}{2}+1-m, m\right)\right\},\ R_{-\alpha}\left(T^*_{\frac{k}{2}-1}\right)\right\} & 10 \leq k \leq 24 \\ \max\left\{\max\limits_{3\leq m\leq 7}\left\{R_{-\alpha}\left(14-m, m\right)\right\},\ R_{-\alpha}\left(T^*_{12}\right)\right\} & k = 26 \\ \max\left\{\max\limits_{3\leq m\leq 6}\left\{R_{-\alpha}\left(\frac{k}{2}+1-m, m\right)\right\},\ R_{-\alpha}\left(T^*_{\frac{k}{2}-1}\right)\right\} & 28 \leq k \leq 30 \\ \max\left\{\max\limits_{3\leq m\leq 5}\left\{R_{-\alpha}\left(\frac{k}{2}+1-m, m\right)\right\},\ R_{-\alpha}\left(T^*_{\frac{k}{2}-1}\right)\right\} & 32 \leq k \leq 142 \\ \max\left\{\max\limits_{3\leq m\leq 4}\left\{R_{-\alpha}\left(\frac{k}{2}+1-m, m\right)\right\},\ R_{-\alpha}\left(T^*_{\frac{k}{2}-1}\right)\right\} & k \geq 144 \end{cases}$$

Proof. We only need to compare the maximum general Randić index $R_{-\alpha}$ of T^0 obtained in **Theorem3.1** and the one of T^1 obtained in **Theorem3.3**. Discuss in two cases based on the parity of order k.

case 1. k is odd

The structure of $T^*_{\frac{k+1}{2}-m,m}$ does not exist when $k \leq 9$, so we only have to consider $k \geq 11$.

Since

$$\begin{aligned} p_m(k,\alpha) &= R_{-\alpha}\left(T_{\frac{k-1}{2}}\right) - R_{-\alpha}\left(T^*_{\frac{k+1}{2}-m,m}\right) \\ &= \frac{1}{2}\left(\frac{1}{(k-1)^{\alpha-1}} - \frac{1}{(k-2m+1)^{\alpha-1}}\right) + \frac{1-\left(\frac{2}{m}\right)^{\alpha}}{(k-2m+1)^{\alpha}} \\ &\quad + \frac{1}{2^{\alpha}} - \frac{1}{4^{\alpha}} - \frac{m-1}{(2m)^{\alpha}} \end{aligned}$$

where $m = 3, 4, 5, 6, 7$.

We should discuss $p_m(k,\alpha)$, $m = 3, 4, 5, 6, 7$ one by one. Take $m = 3$ for instance. Let $H(x,\alpha) = \frac{1}{x^{\alpha-1}}$, then by **Lagrange Mean Value Theorem**,

$$\frac{1}{2}\left(\frac{1}{(k-1)^{\alpha-1}} - \frac{1}{(k-5)^{\alpha-1}}\right) = 2H'(\xi,\alpha)$$

where $\xi \in (k-5, k-1)$.

Notice when $k \geq 13$, $H'(\xi,\alpha) = \frac{1-\alpha}{\xi^\alpha} > \frac{1-\alpha}{8^\alpha}$, then

$$p_3(k,\alpha) > \frac{2(1-\alpha)}{8^\alpha} + \frac{1}{2^\alpha} - \frac{1}{4^\alpha} - \frac{2}{6^\alpha} = S(\alpha)$$

As the proof of $S_1(\alpha) < 0$, we firstly obtain the picture of $S(\alpha)$ in interval $(1,2)$ by mathematica software, and one would see that there is only one root of $S(\alpha) = 0$. Then notice that $S(1.2961) > 0$ and $S(2) > 0$, we conclude that $S(\alpha) > 0$ for $\alpha \in (\alpha_0, 2) \subset (1.2961, 2)$. Hence $p_3(k,\alpha) > S(\alpha) > 0$ for $k \geq 13$. For $k = 11$, we also show $p_3(11,\alpha) > 0$ by the same method. Therefore when $k \geq 11$ is odd, $T_{\frac{k-1}{2}}$ has larger general Randić index than $T^*_{\frac{k+1}{2}-m,m}$ where $m = 3$. Similarly, one may obtain $p_m(k,\alpha) > 0$ for $m = 4,5,6,7$. Consequently, $T_{\frac{k-1}{2}}$ is the Max Tree for odd order k.

case 2. k is even

In this condition, when $k = 8$, the possible structure of the Max Tree is unique, that is T_3^*. But for $k \geq 10$ the structure of the Max Tree has no unique form when α alters. □

Although, there is no unique form of the structure for the Max Tree of even order, when $k \geq 144$ we can define two bounds of α: $\alpha_1^*(k)$ and $\alpha_2^*(k)$ which divide the interval $(\alpha_0, 2)$ into three parts, and in each part the unique form would be obtained.

For $T^*_{\frac{k}{2}-1}$ and $T_{\frac{k}{2}-2,3}$, we have:

$$\begin{aligned} q_1(k,\alpha) &= R_{-\alpha}\left(T^*_{\frac{k}{2}-1}\right) - R_{-\alpha}\left(T_{\frac{k}{2}-2,3}\right) \\ &= \frac{1}{2}\left(\frac{1}{(k-2)^{\alpha-1}} - \frac{1}{(k-4)^{\alpha-1}}\right) + \frac{1-\left(\frac{2}{3}\right)^\alpha}{(k-4)^\alpha} + \frac{1}{4^\alpha} - \frac{2}{6^\alpha} \end{aligned}$$

We see $q_1(+\infty,\alpha) = \frac{1}{4^\alpha} - \frac{2}{6^\alpha} = 0$ has one root $\log_{\frac{3}{2}} 2$.

On the other hand, note the root of equation $q_1(144,\alpha) = 0$ by α_1, it is easy to know $\alpha_1 > \log_{\frac{3}{2}} 2$. Thus by the continuity of $q_1(k,\alpha)$, one may deduce that $\alpha_1^*(k)$ belongs to the interval $\left(\log_{\frac{3}{2}} 2, \alpha_1\right]$. And when $\alpha < \alpha_1^*(k)$, $T_{\frac{k}{2}-2,3}$ has larger general Randić index than $T^*_{\frac{k}{2}-1}$; while $\alpha > \alpha_1^*(k)$, the opposite holds.

For $T_{\frac{k}{2}-2,3}$ and $T_{\frac{k}{2}-3,4}$:

$$\begin{aligned} q_2(k,\alpha) &= R_{-\alpha}\left(T_{\frac{k}{2}-2,3}\right) - R_{-\alpha}\left(T_{\frac{k}{2}-3,4}\right) \\ &= \frac{1}{2}\left(\frac{1}{(k-4)^{\alpha-1}} - \frac{1}{(k-6)^{\alpha-1}}\right) + \frac{1-\left(\frac{1}{2}\right)^\alpha}{(k-6)^\alpha} - \frac{1-\left(\frac{2}{3}\right)^\alpha}{(k-4)^\alpha} \\ &\quad + \frac{2}{6^\alpha} - \frac{3}{8^\alpha} \end{aligned}$$

Function $q_2(+\infty,\alpha) = \frac{2}{6^\alpha} - \frac{3}{8^\alpha} = 0$ has one root $\log_{\frac{4}{3}} \frac{3}{2}$; besides, let the root of $q_2(144,\alpha) = 0$ be α_2, clearly $\alpha_2 > \log_{\frac{4}{3}} \frac{3}{2}$. Thus $\alpha_2^*(k) \in \left(\log_{\frac{4}{3}} \frac{3}{2}, \alpha_2\right]$. When $\alpha < \alpha_2^*(k)$, $T_{\frac{k}{2}-3,4}$ has larger general Randić index than $T_{\frac{k}{2}-2,3}$; while $\alpha > \alpha_2^*(k)$, the opposite holds.

Besides, it is easy to calculate $\alpha_2 < \log_{\frac{3}{2}} 2$, which follows $\alpha_1^*(k) > \alpha_2^*(k)$. So as the sum-up of the above discussion, here is a tabular

$\alpha_0 < \alpha < \alpha_2^*(k)$	$\alpha_2^*(k) < \alpha < \alpha_1^*(k)$	$\alpha_1^*(k) < \alpha < 2$
$T_{\frac{k}{2}-3,4}$	$T_{\frac{k}{2}-2,3}$	$T^*_{\frac{k}{2}-1}$

where $\alpha_0 \in (1.2961, 1.2962), \alpha_1^*(k) \in \left(\log_{\frac{3}{2}} 2, \alpha_1\right], \alpha_2^*(k) \in \left(\log_{\frac{4}{3}} \frac{3}{2}, \alpha_2\right]$.

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