Mathematics

http://www.aimspress.com/journal/Math

AIMS Mathematics, 8(12): 31186–31197.
DOI:10.3934/math.20231596
Received: 15 September 2023
Revised: 13 November 2023
Accepted: 19 November 2023
Published: 23 November 2023

Research article

Higher-order Randić index and isomorphism of double starlike trees

Zhenhua Su[1], Zikai Tang[2] and Hanyuan Deng[2,*]

[1] School of Mathematics and Computational Sciences, Huaihua University, Huaihua, Hunan 418008, China

[2] College of Mathematics and Statistics, Hunan Normal University, Changsha, Hunan 410081, China

* **Correspondence:** Email: hydeng@hunnu.edu.cn.

Abstract: For an integer $h \geq 0$, the hth order Randić index for a simple graph G is defined as $R^h(G) = \sum_\pi \frac{1}{\sqrt{v_1(\pi)v_2(\pi)\cdots v_{h+1}(\pi)}}$, where π extends over all paths of length h in G and $v_i(\pi)$ denotes the degree of the i-th vertex of the path π. In this paper, we showed that the hth order Randić index $R^h(T)$ of a double starlike tree T (a tree with two vertices of degrees $m_1, m_2 > 2$) is completely determined by its branches of length $\leq h$. As a consequence, we proved that the double starlike trees with equal h-Randić index are isomorphic, except for some special values for m_1 and m_2.

Keywords: Randić index; double starlike tree; degree; isomorphism
Mathematics Subject Classification: 05C05, 05C09, 05C92

1. Introduction

In mathematical chemistry, a topological index is a numeric quantity derived mathematically in a direct and unambiguous manner from the structural graph of a molecule, which is used to characterize some properties of a molecular graph. It is also a graph invariant since isomorphic graphs have the same value for a given topological index.

Many topological indices have been developed through the years and related successfully to physicochemical properties of organic molecules [1, 2]. In order to define the concept of branching in molecular species [3, 4], Randić [5] introduced in 1975 a topological index–the connectivity index (now called the Randić index), defined for a simple graph G as

$$R^1(G) = \sum_\pi \frac{1}{\sqrt{v_1(\pi)v_2(\pi)}},$$

where π extends over all paths of length 1 and $v_i(\pi)$ denotes the degree of the i-th vertex of the path π. Note that for a path with $(n + 1)$ vertices and n edges, both of the vertex and edge can appear exactly once. It has become one of the most widely used and most successful in applications to physical and chemical properties [6]. For a review of historical details and a further bibliography on the chemical applications of the Randić index see [7–10].

For an integer $h \geq 0$, the connectivity index of order h (also called h-Randić index) [11] is defined as

$$R^h(G) = \sum_{\pi} \frac{1}{\sqrt{v_1(\pi)v_2(\pi)\cdots v_{h+1}(\pi)}},$$

where π extends over all paths of length h in G and $v_i(\pi)$ denotes the degree of the i-th vertex of the path π.

Higher-order Randić indices are of great interest in the theory of molecular graph theory and some of its mathematical properties have been reported in [12]. Examples of non-isomorphic trees T and T' such that $R^h(T) = R^h(T')$ for all $h \geq 0$ exist [13]. However, it will not occur in starlike trees, i.e. trees that have a unique vertex of a degree greater than 2. In fact, Rada and Araujo [14] proved that starlike trees which have equal h-connectivity index for $h \geq 0$ are isomorphic.

Very recently, by a relation on trees with respect to edge division vectors, Song and Huang [15] found some sufficient conditions to determine whether some trees with the same topological index value are isomorphic or not. Further, several classes of trees, including balanced starlike trees and double star $S_{p,q}$, are uniquely determined by edge division vectors.

This leads naturally to determine h-Randić index of a double starlike tree, i.e., a tree that has only two vertices of a degree greater than 2. In this paper, we will show that for every integer $h \geq 0$, the higher-order Randić $R^h(T)$ of a double starlike tree T is completely determined by its branches of length $\leq h$. As a consequence, we show that almost all the double starlike trees that have equal h-Randić index for all $h \geq 0$ are isomorphic.

2. Some conceptions for double starlike trees

Let G be a graph. The maximum vertex degree and the number of i-vertices (an i-vertex is a vertex of degree i) will be denoted by $\Delta(G)$ and $k_i(G)$, respectively. For an integer $m \geq 2$, a *starlike tree* T is a tree for which $k_1(T) = \Delta(T) = m$. The set of all starlike trees on n vertices with the maximal degree m is denoted by $\Omega_{n,m}$.

For two integers $m_1, m_2 \geq 2$, a *double starlike tree* T is a tree with an edge u_0v_0 such that the components of $T - \{u_0v_0\}$ are two starlike trees T_{u_0} and T_{v_0} with their maximal degrees $m_1 - 1$ and $m_2 - 1$, respectively, where $d_T(u_0) = m_1$ and $d_T(v_0) = m_2$. If $n_1 = |V(T_{u_0})|$ and $n_2 = |V(T_{v_0})|$, then $n_1 + n_2 = n = |V(T)|$. A double starlike tree is displayed as in Figure 1. The set of all double starlike trees on n vertices with two adjacent branching vertices of degrees m_1 and m_2 are denoted by Ω_{n,m_1,m_2}. Specifically, if one of the values m_1 and m_2 is 2, then the double starlike tree is a starlike tree.

For any two vertices u, w in T, we use $[u, w]$ to represent the shortest path connecting u and w, and keep in mind that the number of edges in $[u, w]$ is called the distance. Let $T \in \Omega_{n,m_1,m_2}$. If $\{u_1, u_2, \cdots, u_{m_1-1}\}$ is the set of 1-vertices in T_{u_0}, an l-branch of T_{u_0} is a path $[u_0, u_i]$ of T_{u_0} such that $d(u_0, u_i) = l$. There is a similar definition for T_{v_0}. We denote by $r_l(T)$ and $s_l(T)$ the numbers of l-branches in T_{u_0} and T_{v_0}, respectively (see Figure 1).

Based on the notations introduced above, we clearly have the following relations:

$$r_1 + r_2 + \cdots + r_{t_1} = m_1 - 1, \quad s_1 + s_2 + \cdots + s_{t_2} = m_2 - 1,$$

$$r_1 + 2r_2 + \cdots + t_1 r_{t_1} = n_1 - 1, \quad s_1 + 2s_2 + \cdots + t_2 s_{t_2} = n_2 - 1, \quad n_1 + n_2 = n,$$

where t_1 and t_2 represent the length of the longest branch in T_{u_0} and T_{v_0}, respectively.

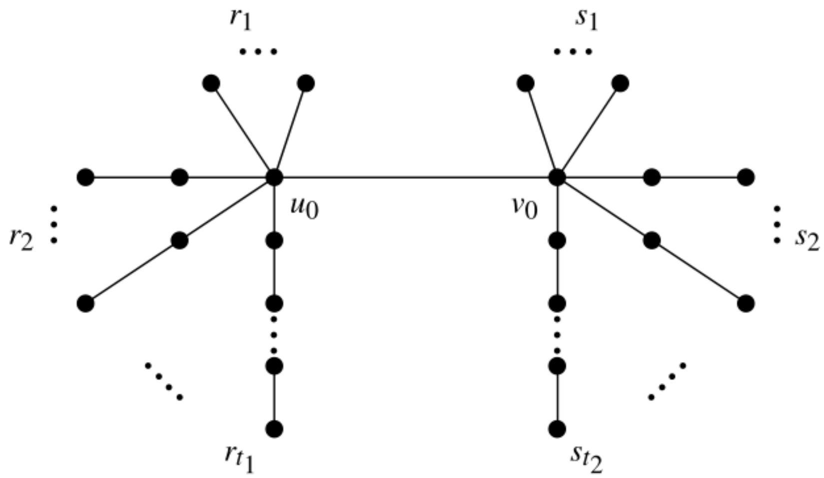

Figure 1. The double starlike tree.

3. Higher-order Randić index for double starlike trees

In this section, we will determine the higher-order Randić index of double starlike trees.

Theorem 3.1. *Let $T \in \Omega_{n,m_1,m_2}$, where $m_1 \neq m_2$. Then*

$$R^0(T) = (m_1 + m_2)(1 - \frac{1}{\sqrt{2}}) + \frac{1}{\sqrt{m_1}} + \frac{1}{\sqrt{m_2}} + \frac{n}{\sqrt{2}} - 2.$$

As a consequence, if $T' \in \Omega_{n,m_1',m_2'}$, then $R^0(T) = R^0(T')$ if and only if $m_1 = m_1'$ and $m_2 = m_2'$.

Proof. It is not difficult to obtain that $k_1(T) = m_1 + m_2 - 2$, $k_2(T) = n - m_1 - m_2$ and $k_{m_1}(T) = k_{m_2}(T) = 1$. Hence,

$$\begin{aligned} R^0(T) &= (m_1 + m_2 - 2) \cdot 1 + (n - m_1 - m_2) \cdot \frac{1}{\sqrt{2}} + \frac{1}{\sqrt{m_1}} + \frac{1}{\sqrt{m_2}} \\ &= (m_1 + m_2)(1 - \frac{1}{\sqrt{2}}) + \frac{1}{\sqrt{m_1}} + \frac{1}{\sqrt{m_2}} + \frac{n}{\sqrt{2}} - 2. \end{aligned}$$

Let $f(m_1, m_2) = (m_1 + m_2)(1 - \frac{1}{\sqrt{2}}) + \frac{1}{\sqrt{m_1}} + \frac{1}{\sqrt{m_2}}$. Clearly, $m_1 + m_2 \in N^+$, and $\frac{1}{\sqrt{m_1}} + \frac{1}{\sqrt{m_2}} \notin N^+$. If $R^0(T) = R^0(T')$, then we have

$$m_1 + m_2 = m_1' + m_2'. \tag{3.1}$$

$$\frac{1}{\sqrt{m_1}} + \frac{1}{\sqrt{m_2}} = \frac{1}{\sqrt{m_1'}} + \frac{1}{\sqrt{m_2'}}. \tag{3.2}$$

In the following, we show that $m_1 = m_1'$ and $m_2 = m_2'$. Assume that $m_1 \neq m_1'$ and $m_2 \neq m_2'$, thus $m_1 \neq m_1' \neq m_2 \neq m_2'$. For convenience, let $a = \sqrt{m_1}$, $b = \sqrt{m_2}$, $c = \sqrt{m_1'}$ and $d = \sqrt{m_2'}$. Without loss of generality, assume $b < d < c < a$. From equations (3.1) and (3.2), it can be concluded that

$$\frac{ac}{db} = \frac{a-c}{d-b}, \quad \frac{a-c}{d-b} = \frac{d+b}{a+c}.$$

Therefore,

$$\frac{ac}{db} = \frac{d+b}{a+c}.$$

On the other hand, according to $b < d < c < a$, we have $ac > bd$ and $a + c > b + d$, i.e.,

$$\frac{ac}{db} > \frac{d+b}{a+c},$$

a contradiction. Therefore, the assumption is not valid and the proof is done. □

In the following, the set of all rational numbers is denoted by Q and the set of all irrational numbers is $R - Q$.

Theorem 3.2. *Let $T \in \Omega_{n,m_1,m_2}$, where $m_1 \neq m_2$. Then*

$$R^1(T) = (\frac{1}{\sqrt{m_1}} - \frac{1}{\sqrt{2m_1}} + \frac{1}{2} - \frac{1}{\sqrt{2}})r_1 + (\frac{1}{\sqrt{m_2}} - \frac{1}{\sqrt{2m_2}} + \frac{1}{2} - \frac{1}{\sqrt{2}})s_1$$
$$+\Big[\frac{m_1+m_2-2}{\sqrt{2}} + \frac{m_1-1}{\sqrt{2m_1}} + \frac{m_2-1}{\sqrt{2m_2}} + \frac{1}{\sqrt{m_1m_2}} - (m_1+m_2) + \frac{n}{2} + 1\Big].$$

Consequently, for $T' \in \Omega_{n,m'_1,m'_2}$, where $m'_1 = m_1$ and $m'_2 = m_2$, if $R^1(T) = R^1(T')$, then
(i) $r_1 = r'_1$ and $s_1 = s'_1$ when $m_1 = 2$ or $m_2 = 2$;
(ii) $r_1 = r'_1$ and $s_1 = s'_1$, except for the case $\sqrt{m_1}, \sqrt{m_2} \in R-Q$ and $\sqrt{2m_1}, \sqrt{2m_2} \in Q$, when $m_1, m_2 \geq 3$.

Proof. Note that $\frac{1}{2}\sum_{i=r_1+1}^{m_1-1} d(u_0, u_i) + \frac{1}{2}\sum_{i=s_1+1}^{m_2-1} d(v_0, v_i) = \frac{1}{2}(n - r_1 - s_1 - 2)$. Keeping the notation of $R^1(T)$, we have

$$R^1(T) = \sum_{i=1}^{r_1}\frac{1}{\sqrt{m_1}} + \sum_{i=r_1+1}^{m_1-1}\Big[\frac{1}{\sqrt{2}} + \frac{1}{2}(d(u_0,u_i)-2) + \frac{1}{\sqrt{2m_1}}\Big]$$
$$+ \sum_{i=1}^{s_1}\frac{1}{\sqrt{m_2}} + \sum_{i=s_1+1}^{m_2-1}\Big[\frac{1}{\sqrt{2}} + \frac{1}{2}(d(v_0,v_i)-2) + \frac{1}{\sqrt{2m_2}}\Big] + \frac{1}{\sqrt{m_1m_2}}$$
$$= (\frac{1}{\sqrt{m_1}} - \frac{1}{\sqrt{2m_1}} + \frac{1}{2} - \frac{1}{\sqrt{2}})r_1 + (\frac{1}{\sqrt{m_2}} - \frac{1}{\sqrt{2m_2}} + \frac{1}{2} - \frac{1}{\sqrt{2}})s_1 + \lambda(n, m_1, m_2),$$

where $\lambda(n, m_1, m_2) = \Big[\frac{m_1+m_2-2}{\sqrt{2}} + \frac{m_1-1}{\sqrt{2m_1}} + \frac{m_2-1}{\sqrt{2m_2}} + \frac{1}{\sqrt{m_1m_2}} - (m_1+m_2) + \frac{n}{2} + 1\Big]$.

For convenience, let $a = (\frac{1}{\sqrt{m_1}} - \frac{1}{\sqrt{2m_1}} + \frac{1}{2} - \frac{1}{\sqrt{2}})$, and $b = (\frac{1}{\sqrt{m_2}} - \frac{1}{\sqrt{2m_2}} + \frac{1}{2} - \frac{1}{\sqrt{2}})$.

(i) If one of m_1 and m_2 is 2, assume that $m_1 = 2$. Then $R^1(T) = ar_1 + bs_1 + \lambda(n, m_1, m_2)$. We can immediately deduce $s_1 = s'_1$ from the condition $R^1(T) = R^1(T')$. In this case, we have $r_1 = r'_1 = 1$ and $a = 0$.

(ii) If $m_1, m_2 \geq 3$, from $R^1(T) = R^1(T')$, we obtain that $ar_1 + bs_1 = ar'_1 + bs'_1$. If $r_1 = r'_1$(or $s_1 = s'_1$), then we can obtain that $s_1 = s'_1$ (or $r_1 = r'_1$), the theorem is true. In the following, we will deduce a contradiction under the assumption of $r_1 \neq r'_1$ and $s_1 \neq s'_1$. Denote

$$\frac{a}{b} = \frac{s'_1 - s_1}{r_1 - r'_1} = t. \tag{3.3}$$

Let's discuss in three cases according to whether $\sqrt{m_1}$ and $\sqrt{m_2}$ are rational numbers.

Case 1. $\sqrt{m_1} = c \in Q$ and $\sqrt{m_2} = d \in Q$.

From Equation (3.3), it can be concluded that

$$\frac{a}{b} = \frac{\frac{1}{c} - \frac{1}{c\sqrt{2}} + \frac{1}{2} - \frac{1}{\sqrt{2}}}{\frac{1}{d} - \frac{1}{d\sqrt{2}} + \frac{1}{2} - \frac{1}{\sqrt{2}}} = t,$$

and we get $t = \frac{d(c+2)}{c(d+2)} = \frac{d(c+1)}{c(d+1)}$. Furthermore, we have $c = d$, i.e., $m_1 = m_2$, which contradicts with $m_1 \neq m_2$.

Case 2. $\sqrt{m_1} = c \in Q$ and $\sqrt{m_2} \in R - Q$.

Subcase 2.1. $\sqrt{2m_2} = d \in Q$.

From Equation (3.3), it can be concluded that

$$\frac{a}{b} = \frac{\frac{1}{c} - \frac{1}{c\sqrt{2}} + \frac{1}{2} - \frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{m_2}} - \frac{1}{d} + \frac{1}{2} - \frac{1}{\sqrt{2}}} = t.$$

Thus, we get $t = \frac{d(c+2)}{c(d-2)} = \frac{d(c+1)}{c(d-2)}$, i.e., $c + 1 = c + 2$, a contradiction.

Subcase 2.2. $\sqrt{2m_2} \in R - Q$.

By Equation (3.3), we obtain

$$\frac{a}{b} = \frac{\frac{1}{c} - \frac{1}{c\sqrt{2}} + \frac{1}{2} - \frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{m_2}} - \frac{1}{\sqrt{2m_2}} + \frac{1}{2} - \frac{1}{\sqrt{2}}} = t,$$

and we have $t = \frac{c+2}{c} = \frac{-\sqrt{m_2}(c+1)}{(\sqrt{2} - \sqrt{m_2} - 1)c}$, which implies $\sqrt{2}(2 + c) - \sqrt{m_2} - (2 + c) = 0$, i.e., $c = -2$ and $m_2 = 0$, a contradiction.

Case 3. $\sqrt{m_1} \in R - Q$, $\sqrt{m_2} \in R - Q$.

Subcase 3.1. $\sqrt{2m_1} = c \in Q$, $\sqrt{2m_2} \in R - Q$.

By Equation (3.3), we obtain

$$\frac{a}{b} = \frac{\frac{1}{\sqrt{m_1}} - \frac{1}{c} + \frac{1}{2} - \frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{m_2}} - \frac{1}{\sqrt{2m_2}} + \frac{1}{2} - \frac{1}{\sqrt{2}}} = t.$$

Then we have $t = \frac{c-2}{c} = \frac{\sqrt{2m_2}(\sqrt{2} - \sqrt{m_1})}{c(\sqrt{2} - \sqrt{m_2} - 1)}$, i.e., $m_1 = 2$, which contradicts with $m_1 \geq 3$.

Subcase 3.2. $\sqrt{2m_1} \in R - Q$, $\sqrt{2m_2} \in R - Q$.

By Equation (3.3), we obtain

$$\frac{a}{b}=\frac{\frac{1}{\sqrt{m_1}}-\frac{1}{\sqrt{2m_1}}+\frac{1}{2}-\frac{1}{\sqrt{2}}}{\frac{1}{\sqrt{m_2}}-\frac{1}{\sqrt{2m_2}}+\frac{1}{2}-\frac{1}{\sqrt{2}}}=t.$$

Similarly, it can be concluded that $t=1=\frac{\frac{1}{\sqrt{m_1}}-\frac{1}{\sqrt{2m_1}}}{\frac{1}{\sqrt{m_2}}-\frac{1}{\sqrt{2m_2}}}$, i.e., $m_1=m_2$, which contradicts with $m_1\neq m_2$.

Therefore, taking into account the above situations, we obtain that $r_1=r_1'$ and $s_1=s_1'$, except for the case $\sqrt{m_1}$, $\sqrt{m_2}\in R-Q$ and $\sqrt{2m_1}$, $\sqrt{2m_2}\in Q$. □

Next, We will extend this result to $R^h(T)$, where $h\geq 2$.

Let u_0 and v_0 be the m_1-vertex and m_2-vertex of T (see Figure 1). Let P_h represent the set of all paths of length h in T, $N=\{0,1,2,\cdots\}$ as the set of natural numbers and the function $\Psi: P_h\longrightarrow N^{h+1}$ by $\Psi(\pi)=(v_1(\pi),\cdots,v_{h+1}(\pi))$, where $v_i(\pi)$ denotes the degree of the i-th vertex of the path π.

We first consider all paths in P_h that contain u_0 or v_0 as an end-vertex, or do not contain u_0 and v_0. There are twelve possibilities for the images under Ψ of these paths:

$$X_1=(1,\underbrace{2,\cdots,2}_{h-1},m_1),\quad X_1'=(1,\underbrace{2,\cdots,2}_{h-1},m_2),$$
$$X_2=(\underbrace{2,\cdots,2}_{h},m_1),\quad X_2'=(\underbrace{2,\cdots,2}_{h},m_2),$$
$$X_3=(\underbrace{2,\cdots,2}_{h+1}),\quad X_3'=(\underbrace{2,\cdots,2}_{h+1}),$$
$$X_4=(1,\underbrace{2,\cdots,2}_{h}),\quad X_4'=(1,\underbrace{2,\cdots,2}_{h}),$$
$$X_5=(1,\underbrace{2,\cdots,2}_{h-2},m_1,m_2),\quad X_5'=(1,\underbrace{2,\cdots,2}_{h-2},m_2,m_1),$$
$$X_6=(\underbrace{2,\cdots,2}_{h-1},m_1,m_2),\quad X_6'=(\underbrace{2,\cdots,2}_{h-1},m_2,m_1).$$

We then consider all paths in P_h that contain only one of u_0 and v_0, but not as an end-vertex. In this case the image of Ψ is as follows:

$Y_1(a)=(1,\underbrace{2,\cdots,2}_{a},m_1,\underbrace{2,\cdots,2}_{h-1-a})$, $Y_1'(a)=(1,\underbrace{2,\cdots,2}_{a},m_2,\underbrace{2,\cdots,2}_{h-1-a})$, where $0\leq a\leq h-2$.

$Y_2(a)=(1,\underbrace{2,\cdots,2}_{a},m_1,\underbrace{2,\cdots,2}_{h-2-a},1)$, $Y_2'(a)=(1,\underbrace{2,\cdots,2}_{a},m_2,\underbrace{2,\cdots,2}_{h-2-a},1)$, where $0\leq a\leq\frac{h}{2}-1$.

$Y_3(a)=(\underbrace{2,\cdots,2}_{a},m_1,\underbrace{2,\cdots,2}_{h-a})$, $Y_3'(a)=(\underbrace{2,\cdots,2}_{a},m_2,\underbrace{2,\cdots,2}_{h-a})$, where $1\leq a\leq\frac{h}{2}$.

Finally, consider all paths in P_h that contain both v_0 and u_0, but not one as an end-vertex. In this case the image of Ψ is as follows:

$Z_1(a)=(1,\underbrace{2,\cdots,2}_{a},m_1,m_2,\underbrace{2,\cdots,2}_{h-2-a})$, $Z_1'(a)=(1,\underbrace{2,\cdots,2}_{a},m_2,m_1,\underbrace{2,\cdots,2}_{h-2-a})$, where $0\leq a\leq h-3$.

$Z_2(a)=(1,\underbrace{2,\cdots,2}_{a},m_1,m_2,\underbrace{2,\cdots,2}_{h-3-a},1)$, where $0\leq a\leq h-3$.

$Z_3(a)=(\underbrace{2,\cdots,2}_{a},m_1,m_2,\underbrace{2,\cdots,2}_{h-1-a})$, where $1\leq a\leq h-2$.

Now, let's prove our main result.

Theorem 3.3. *Let $T \in \Omega_{n,m_1,m_2}$, where $m_1 \neq m_2$. Then*

$$R^h(T) = (\frac{1}{\sqrt{2^{h-1}m_1}} - \frac{1}{\sqrt{2^h m_1}} + \frac{1}{\sqrt{2^{h+1}}} - \frac{1}{\sqrt{2^h}})r_h + (\frac{1}{\sqrt{2^{h-1}m_2}} - \frac{1}{\sqrt{2^h m_2}} + \frac{1}{\sqrt{2^{h+1}}} - \frac{1}{\sqrt{2^h}})s_h + \lambda(h, n, m_1, m_2, r_1, s_1, \cdots, r_{h-1}, s_{h-1}),$$

where $\lambda(h, n, m_1, m_2, r_1, s_1, \cdots, r_{h-1}, s_{h-1})$ is a real number determined by the values of $h, n, m_1, m_2, \cdots, r_{h-1}, s_{h-1}$.

Proof. Clearly, $R^h(T)$ is determined by the numbers $|\Psi^{-1}(X_i)|$, $|\Psi^{-1}(X'_i)|$, $|\Psi^{-1}(Y_i(a))|$, $|\Psi^{-1}(Y'_i(a))|$, $|\Psi^{-1}(Z_i(a))|$ and $|\Psi^{-1}(Z'_i(a))|$, where $|\Psi^{-1}(W)|$ represents the number of elements in the inverse image of W under Ψ, i.e.,

$$\begin{aligned} R^h(T) = {} & |\Psi^{-1}(X_1)|\frac{1}{\sqrt{2^{h-1}m_1}} + |\Psi^{-1}(X'_1)|\frac{1}{\sqrt{2^{h-1}m_2}} + |\Psi^{-1}(X_2)|\frac{1}{\sqrt{2^h m_1}} + |\Psi^{-1}(X'_2)|\frac{1}{\sqrt{2^h m_2}} \\ & + |\Psi^{-1}(X_3)|\frac{1}{\sqrt{2^{h+1}}} + |\Psi^{-1}(X'_3)|\frac{1}{\sqrt{2^{h+1}}} + |\Psi^{-1}(X_4)|\frac{1}{\sqrt{2^h}} + |\Psi^{-1}(X'_4)|\frac{1}{\sqrt{2^h}} \\ & + |\Psi^{-1}(X_5)|\frac{1}{\sqrt{2^{h-2}m_1m_2}} + |\Psi^{-1}(X'_5)|\frac{1}{\sqrt{2^{h-2}m_1m_2}} + |\Psi^{-1}(X_6)|\frac{1}{\sqrt{2^{h-1}m_1m_2}} \\ & + |\Psi^{-1}(X'_6)|\frac{1}{\sqrt{2^{h-1}m_1m_2}} + \sum_{a=0}^{h-2}|\Psi^{-1}(Y_1(a))|\frac{1}{\sqrt{2^{h-1}m_1}} + \sum_{a=0}^{h-2}|\Psi^{-1}(Y'_1(a))|\frac{1}{\sqrt{2^{h-1}m_2}} \\ & + \sum_{a=0}^{\frac{h}{2}-1}|\Psi^{-1}(Y_2(a))|\frac{1}{\sqrt{2^{h-2}m_1}} + \sum_{a=0}^{\frac{h}{2}-1}|\Psi^{-1}(Y'_2(a))|\frac{1}{\sqrt{2^{h-2}m_2}} + \sum_{a=1}^{\frac{h}{2}}|\Psi^{-1}(Y_3(a))|\frac{1}{\sqrt{2^h m_1}} \\ & + \sum_{a=1}^{\frac{h}{2}}|\Psi^{-1}(Y'_3(a))|\frac{1}{\sqrt{2^h m_2}} + \sum_{a=0}^{h-3}|\Psi^{-1}(Z_1(a))|\frac{1}{\sqrt{2^{h-2}m_1m_2}} + \sum_{a=0}^{h-3}|\Psi^{-1}(Z'_1(a))|\frac{1}{\sqrt{2^{h-2}m_1m_2}} \\ & + \sum_{a=0}^{h-3}|\Psi^{-1}(Z_2(a))|\frac{1}{\sqrt{2^{h-3}m_1m_2}} + \sum_{a=1}^{h-2}|\Psi^{-1}(Z_3(a))|\frac{1}{\sqrt{2^{h-1}m_1m_2}}. \end{aligned}$$

We can express $|\Psi^{-1}(X_i)|$, $|\Psi^{-1}(X'_i)|$, $|\Psi^{-1}(Y_i(a))|$, $|\Psi^{-1}(Y'_i(a))|$, $|\Psi^{-1}(Z_i(a))|$ and $|\Psi^{-1}(Z'_i(a))|$ in terms of $r_1, s_1, \cdots, r_h, s_h$ by a counting argument together with the reduction formulas as follows:

$$|\Psi^{-1}(X_1)| = r_h, \quad |\Psi^{-1}(X'_1)| = s_h,$$

$$|\Psi^{-1}(X_2)| = r_{h+1} + \cdots + r_{t_1} = m_1 - 1 - \sum_{i=1}^{h} r_i, \quad |\Psi^{-1}(X'_2)| = m_2 - 1 - \sum_{i=1}^{h} s_i,$$

$$\begin{aligned} |\Psi^{-1}(X_3)| &= r_{h+1} + 2r_{h+2} + \cdots + (t-h-1)r_{t_1} = -(h+1)\sum_{i=h+1}^{t_1} r_i + \sum_{i=h+1}^{t_1} ir_i, \\ &= -(h+1)\Big[m_1 - 1 - \sum_{i=1}^{h} r_i\Big] + \Big[n_1 - 1 - \sum_{i=1}^{h} ir_i\Big], \end{aligned}$$

$$|\Psi^{-1}(X_3')| = -(h+1)\Big[m_2 - 1 - \sum_{i=1}^{h} s_i\Big] + \Big[n_2 - 1 - \sum_{i=1}^{h} i s_i\Big],\ \text{where } n_1 + n_2 = n,$$

$$|\Psi^{-1}(X_4)| = m_1 - 1 - \sum_{i=1}^{h} r_i,\ \ |\Psi^{-1}(X_4')| = m_2 - 1 - \sum_{i=1}^{h} s_i,$$

$$|\Psi^{-1}(X_5)| = r_{h-1},\ \ |\Psi^{-1}(X_5')| = s_{h-1},$$

$$|\Psi^{-1}(X_6)| = r_h + \cdots + r_{t_1} = m_1 - 1 - \sum_{i=1}^{h-1} r_i,\ \ |\Psi^{-1}(X_6')| = m_1 - 1 - \sum_{i=1}^{h-1} s_i,$$

$$|\Psi^{-1}(Y_1(a))| = \begin{cases} r_{a+1}(m_1 - 1 - \sum_{i=1}^{h-1-a} r_i), & \text{if } 0 \le a < \frac{h-1}{2}, \\ r_{a+1}(m_1 - 2 - \sum_{i=1}^{h-1-a} r_i), & \text{if } \frac{h-1}{2} \le a \le h-2. \end{cases}$$

$$|\Psi^{-1}(Y_1'(a))| = \begin{cases} s_{a+1}(m_2 - 1 - \sum_{i=1}^{h-1-a} s_i), & \text{if } 0 \le a < \frac{h-1}{2}, \\ s_{a+1}(m_2 - 2 - \sum_{i=1}^{h-1-a} s_i), & \text{if } \frac{h-1}{2} \le a \le h-2. \end{cases}$$

$$|\Psi^{-1}(Y_2(a))| = \begin{cases} r_{a+1} r_{h-1-a}, & \text{if } 0 \le a < \frac{h}{2} - 1, \\ \frac{1}{2} r_{a+1}(r_{a+1} - 1), & \text{if } a = \frac{h}{2} - 1. \end{cases}$$

$$|\Psi^{-1}(Y_2'(a))| = \begin{cases} s_{a+1} s_{h-1-a}, & \text{if } 0 \le a < \frac{h}{2} - 1, \\ \frac{1}{2} s_{a+1}(s_{a+1} - 1), & \text{if } a = \frac{h}{2} - 1. \end{cases}$$

$$|\Psi^{-1}(Y_3(a))| = \begin{cases} \Big[m_1 - 1 - \sum_{i=1}^{h-a} r_i\Big]\Big[m_1 - 2 - \sum_{i=1}^{a} r_i\Big], & \text{if } 1 \le a \le \frac{h-1}{2}, \\ \frac{1}{2}\Big[m_1 - 1 - \sum_{i=1}^{h-a} r_i\Big]\Big[m_1 - 2 - \sum_{i=1}^{a} r_i\Big], & \text{if } a = \frac{h}{2}. \end{cases}$$

$$|\Psi^{-1}(Y_3'(a))| = \begin{cases} \Big[m_2 - 1 - \sum_{i=1}^{h-a} s_i\Big]\Big[m_2 - 2 - \sum_{i=1}^{a} s_i\Big], & \text{if } 1 \le a \le \frac{h-1}{2}, \\ \frac{1}{2}\Big[m_2 - 1 - \sum_{i=1}^{h-a} s_i\Big]\Big[m_2 - 2 - \sum_{i=1}^{a} s_i\Big], & \text{if } a = \frac{h}{2}. \end{cases}$$

$$|\Psi^{-1}(Z_1(a))| = r_{a+1}\Big(m_2 - 1 - \sum_{i=1}^{h-2-a} s_i\Big),\ \ \text{if } 0 \le a \le h-3,$$

$$|\Psi^{-1}(Z_1'(a))| = s_{a+1}\Big(m_1 - 1 - \sum_{i=1}^{h-2-a} r_i\Big),\ \ \text{if } 0 \le a \le h-3,$$

$$|\Psi^{-1}(Z_2(a))| = r_{a+1}s_{h-2-a}, \ \text{ if } 0 \le a \le h-3,$$

$$|\Psi^{-1}(Z_3(a))| = \Big(m_1 - 1 - \sum_{i=1}^{a} r_i\Big)\Big(m_2 - 1 - \sum_{i=1}^{h-1-a} s_i\Big), \ \text{ if } 1 \le a \le h-2.$$

We can see that $|\Psi^{-1}(X_i)|$, $|\Psi^{-1}(X'_i)|$, $|\Psi^{-1}(Y_j(a))|$, $|\Psi^{-1}(Y'_j(a))|$, $|\Psi^{-1}(Z_j(a))|$ and $|\Psi^{-1}(Z'_j(a))|$ depend on the numbers $h, m, r_1, s_1, \cdots, r_{h-1}, s_{h-1}$ for all a and $i = 5, 6$ and $j = 1, 2, 3$; while for $i = 1, 2, 3, 4$, $|\Psi^{-1}(X_i)|$ and $|\Psi^{-1}(X'_i)|$ depend on the numbers $h, m, r_1, s_1, \cdots, r_h, s_h$. Hence, by grouping in a convenient way we can get

$$R^h(T) = \lambda(h, n, m_1, m_2, r_1, s_1, \cdots, r_{h-1}, s_{h-1}) + \mu(h, m_1, m_2, r_h, s_h),$$

where $\lambda(h, n, m_1, m_2, r_1, s_1, \cdots, r_{h-1}, s_{h-1})$ is a real number determined by the values of h, n, m_1, $m_2, r_1, s_1, \cdots, r_{h-1}, s_{h-1}$, and

$$\begin{aligned}\mu(h, m_1, m_2, r_h, s_h) = &\Big(\frac{1}{\sqrt{2^{h-1}m_1}} - \frac{1}{\sqrt{2^h m_1}} + \frac{1}{\sqrt{2^{h+1}}} - \frac{1}{\sqrt{2^h}}\Big)r_h \\ &+ \Big(\frac{1}{\sqrt{2^{h-1}m_2}} - \frac{1}{\sqrt{2^h m_2}} + \frac{1}{\sqrt{2^{h+1}}} - \frac{1}{\sqrt{2^h}}\Big)s_h.\end{aligned}$$

Thus, the theorem holds. □

Example 3.4. Let $T \in \Omega_{18,7,4}$ with $r_1(T) = 3$, $r_2(T) = 2$, $r_3(T) = 1$, $s_1(T) = 2$ and $s_4(T) = 1$, where $m_1 = 7, m_2 = 4$. In order to calculate $R^3(T)$, we first determine the number of paths of each type:

$$|\Psi^{-1}(X_1)| = r_3 = 1, \ |\Psi^{-1}(X'_1)| = s_3 = 0,$$

$$|\Psi^{-1}(X_2)| = m_1 - 1 - \sum_{i=1}^{3} r_i = 0, \ |\Psi^{-1}(X'_2)| = 1,$$

$$|\Psi^{-1}(X_3)| = -(3+1)\Big[m_1 - 1 - \sum_{i=1}^{3} r_i\Big] + \Big[n_1 - 1 - \sum_{i=1}^{3} i r_i\Big] = 0, \ |\Psi^{-1}(X'_3)| = 0,$$

$$|\Psi^{-1}(X_4)| = m_1 - 1 - \sum_{i=1}^{3} r_i = 0, \ |\Psi^{-1}(X'_4)| = 1,$$

$$|\Psi^{-1}(X_5)| = r_2 = 2, \ |\Psi^{-1}(X'_5)| = s_2 = 0,$$

$$|\Psi^{-1}(X_6)| = m_1 - 1 - \sum_{i=1}^{2} r_i = 1, \ |\Psi^{-1}(X'_6)| = 1,$$

$$|\Psi^{-1}(Y_1(0))| = r_1(m_1 - 1 - \sum_{i=1}^{2} r_i) = 3, \ |\Psi^{-1}(Y_1(1))| = r_2(m_1 - 2 - r_1) = 4,$$

$$|\Psi^{-1}(Y'_1(0))| = s_1(m_2 - 1 - \sum_{i=1}^{2} s_i) = 2, |\Psi^{-1}(Y'_1(1))| = s_2(m_2 - 2 - s_1) = 0,$$

$$|\Psi^{-1}(Y_2(0))| = r_1 r_2 = 6, \ |\Psi^{-1}(Y'_2(0))| = 0,$$

$$|\Psi^{-1}(Y_3(1))| = \Big[m_1 - 1 - \sum_{i=1}^{2} r_i\Big]\Big[m_1 - 2 - r_1\Big] = 2, \ |\Psi^{-1}(Y'_3(1))| = 0,$$

$$|\Psi^{-1}(Z_1(0))| = r_1(m_2 - 1 - s_1) = 3, \ \ |\Psi^{-1}(Z_1'(0))| = s_1(m_1 - 1 - r_1) = 6,$$
$$|\Psi^{-1}(Z_2(0))| = r_1 s_1 = 6, \ \ |\Psi^{-1}(Z_3(1))| = (m_1 - 1 - r_1)(m_2 - 1 - s_1) = 3.$$

Hence, we obtain from Theorem 3.3

$$\begin{aligned} R^3(T) = &\frac{1}{\sqrt{28}} + 0\frac{1}{\sqrt{16}} + 0\frac{1}{\sqrt{56}} + 1\frac{1}{\sqrt{32}} + 0\frac{1}{\sqrt{16}} + 0\frac{1}{\sqrt{16}} + 0\frac{1}{\sqrt{8}} + \frac{1}{\sqrt{8}} + 2\frac{1}{\sqrt{56}} \\ &+ 0\frac{1}{\sqrt{56}} + \frac{1}{\sqrt{112}} + \frac{1}{\sqrt{112}} + (3+4)\frac{1}{\sqrt{28}} + (2+0)\frac{1}{\sqrt{16}} + 6\frac{1}{\sqrt{14}} + 0\frac{1}{\sqrt{8}} \\ &+ 2\frac{1}{\sqrt{56}} + 0\frac{1}{\sqrt{32}} + 3\frac{1}{\sqrt{56}} + 6\frac{1}{\sqrt{56}} + 6\frac{1}{\sqrt{28}} + 3\frac{1}{\sqrt{112}} \\ = &\frac{1}{2} + \frac{1}{2\sqrt{2}} + \frac{1}{4\sqrt{2}} + (7 + \frac{5}{4})\frac{1}{\sqrt{7}} + (6 + \frac{13}{2})\frac{1}{\sqrt{14}}. \end{aligned}$$ □

Theorem 3.5. *Let $T, T' \in \Omega_{n,m_1,m_2}$, where $m_1 \neq m_2$. Then T and T' are isomorphic if and only if*
(i) $R^h(T) = R^h(T')$ for all $h \geq 0$, where $min\{m_1, m_2\} = 2$; or
(ii) $R^h(T) = R^h(T')$ for all $h \geq 0$, where $m_1, m_2 \geq 3$, except for the case $\sqrt{m_1}, \sqrt{m_2} \in R - Q$ and $\sqrt{2m_1}, \sqrt{2m_2} \in Q$.

Proof. The necessity is clear, we only need to prove sufficiency. Assume that $T, T' \in \Omega_{n,m_1,m_2}$. Since $R^0(T) = R^0(T')$, by Theorem 3.1, $m_1 = m_1'$ and $m_2 = m_2'$. Now, from $R^1(T) = R^1(T')$ and Theorem 3.2, we have $r_1 = r_1'$ and $s_1 = s_1'$, where $min\{m_1, m_2\} = 2$, or where $m_1, m_2 \geq 3$, except for the case $\sqrt{m_1}, \sqrt{m_2} \in R - Q$ and $\sqrt{2m_1}, \sqrt{2m_2} \in Q$. Next, applying Theorem 3.3 for $h = 2$, we get

$$\begin{aligned} &(\frac{1}{\sqrt{2^1 m_1}} - \frac{1}{\sqrt{2^2 m_1}} + \frac{1}{\sqrt{2^3}} - \frac{1}{\sqrt{2^2}})r_2 + (\frac{1}{\sqrt{2^1 m_2}} - \frac{1}{\sqrt{2^2 m_2}} + \frac{1}{\sqrt{2^3}} - \frac{1}{\sqrt{2^2}})s_2 + \lambda \\ &= (\frac{1}{\sqrt{2^1 m_1}} - \frac{1}{\sqrt{2^2 m_1}} + \frac{1}{\sqrt{2^3}} - \frac{1}{\sqrt{2^2}})r_2' + (\frac{1}{\sqrt{2^1 m_2}} - \frac{1}{\sqrt{2^2 m_2}} + \frac{1}{\sqrt{2^3}} - \frac{1}{\sqrt{2^2}})s_2' + \lambda \end{aligned}$$

i.e.,

$$\begin{aligned} &(\frac{1}{\sqrt{m_1}} - \frac{1}{\sqrt{2m_1}} + \frac{1}{2} - \frac{1}{\sqrt{2}})r_2 + (\frac{1}{\sqrt{m_2}} - \frac{1}{\sqrt{2m_2}} + \frac{1}{2} - \frac{1}{\sqrt{2}})s_2 \\ &= (\frac{1}{\sqrt{m_1}} - \frac{1}{\sqrt{2m_1}} + \frac{1}{2} - \frac{1}{\sqrt{2}})r_2' + (\frac{1}{\sqrt{m_2}} - \frac{1}{\sqrt{2m_2}} + \frac{1}{2} - \frac{1}{\sqrt{2}})s_2' \end{aligned}$$

By a proof process similar to Theorem 3.2, we have $r_2 = r_2'$ and $s_2 = s_2'$. Continuing this process by repeated use of Theorem 3.3 and Theorem 3.2, we can conclude that $r_i = r_i'$ and $s_i = s_i'$ for all $i \in N$. Therefore, T and T' are isomorphic. □

Finally, let $T \in \Omega_{n,m_1,m_2}$. If $min\{m_1, m_2\} = 2$, then T is a starlike tree, i.e., $T \in \Omega_{n,m}$, where $m = max\{m_1, m_2\}$. From Theorem 3.3 and Theorem 3.5, we have the following corollaries which are given in [14].

Corollary 3.6. [14] *Let $T \in \Omega_{n,m}$. Then*

$$R^h(T) = (\frac{1}{\sqrt{2^{h-1}m}} - \frac{1}{\sqrt{2^h m}} + \frac{1}{\sqrt{2^{h+1}}} - \frac{1}{\sqrt{2^h}})s_h + \lambda(h, n, m, s_1, \cdots, s_{h-1}),$$

where $\lambda(h, n, m, s_1, \cdots, s_{h-1})$ is a real number determined by the values of $h, n, m, s_1, \cdots, s_{h-1}$.

Corollary 3.7. [14] *Let $T, T' \in \Omega_{n,m}$. Then T and T' are isomorphic if and only if $R^h(T) = R^h(T')$ for all $h \geq 0$.*

4. Conclusions

In this paper, we mainly investigated the hth order Randić index $R^h(T)$ of the double starlike tree T, which is a tree with two vertices of degrees $m_1, m_2 > 2$. First, the formula of the hth order Randić index $R^h(T)$ has been completely determined by its branches of length $\leq h$. Second, it was taken that $m_1 \neq m_2$, and we have shown that almost all the double starlike trees $T \in \Omega_{n,m_1,m_2}$ with equal h-Randić index for all $h \geq 0$ are isomorphic. In addition, some results of starlike trees have been obtained, which were given in [14].

These results lead to a natural question, which we pose as a problem.

Problem 3.8. *Which index can determine isomorphism of double starlike trees $T \in \Omega_{n,m_1,m_2}$, where $m_1 = m_2$?*

Use of AI tools declaration

The authors declare they have not used Artificial Intelligence (AI) tools in the creation of this article.

Acknowledgments

This work is supported by the Department of Education of Hunan Province (22B0763), (22B0828), the National Natural Science Foundation of China (12201634), and the Natural Science Foundation of Hunan Province (2023JJ30070).

Conflict of interest

The authors declare that they have no conflicts of interest.

References

1. D. Plavaic, S. Nikolic, N. Trinajstic, Z. Mihalic, On the Harary index for the characterization of chemical graphs, *J. Math. Chem.,* **12** (1993), 235–250. https://doi.org/10.1007/BF01164638
2. N. Ghareghani, F, Ramezani, B. Tayfeh-Rezaie, Graphs cospectral with starlike trees, *Lin. Alg. Appl.,* **429** (2008), 2691–2701. https://doi.org/10.1016/j.laa.2008.01.001
3. O. Araujo, J. A. de la Peña, The connectivity index of a weighted graph, *Lin. Alg. Appl.,* **283** (1998), 171–177. https://doi.org/10.1016/S0024-3795(98)10096-4
4. I. Gutman, M. Randić, Algebraic characterization of skeletal branching, *Chem. Phys. Lett.,* **47** (1977), 15–19. https://doi.org/10.1016/0009-2614(77)85296-2
5. M. Randić, On the characterization of molecular branching, *J. Am. Chem. Soc.,* **97** (1975), 6609–6615.

6. L. B. Kier, L. H. Hall, Molecular connectivity in structure-activity analysis, New York: Wiley Press, 1986.

7. J. Du, Y. Shao, X. Sun, The zeroth-order general Randić index of graph with a given clique number, *Korean J. Math.,* **28** (2020), 405–419. https://doi.org/10.11568/KJM.2020.28.3.405

8. I. Gutman, Some less familiar properties of Randić index, *Croatica Chemica Acta,* **93** (2021), 273–278. https://doi.org/10.5562/cca3747

9. B. Furtula, A. Graovac, D, Vukicevic, Atom-bond connectivity index of trees, *Discrete Appl. Math.,* **157** (2009), 2828–2835. https://doi.org/10.1016/j.dam.2009.03.004

10. L. Volkmann, Sufficient conditions on the zeroth-order general Randić index for maximally edge-connected digraphs, *Communications in Combinatorics and Optimization,* **1** (2016), 1–13.

11. I. G. Yero, J. A. Rodríguez-Velázquez, I. Guyman, Estimating the higher-order Randić index, *Chem. Phys. Lett.,* **489** (2010), 118–120. https://doi.org/10.1016/j.cplett.2010.02.052

12. O. Araujo, J. Rada, Randić index and lexicographic order, *J. Math. Chem.,* **27** (2000), 201–212. https://doi.org/10.1023/A:1026424219580

13. M. Randić, Representation of molecular graphs by basic graphs, *J. Chem. Inf. Comput. Sci.,* **32** (1992), 57–69. https://doi.org/10.1021/ci00005a010

14. J. Rada, O. Araujo, Higher order connectivity index of starlike trees, *Discrete Appl. Math.,* **119** (2002), 287–295. https://doi.org/10.1016/S0166-218X(01)00232-3

15. R. Song, Q. Huang, A relation on trees and the topological indices based on subgraph, *MATCH Commun. Math. Comput. Chem.,* **89** (2023), 343–370. https://doi.org/10.46793/match.89-2.343S

AIMS Press